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The structure of octachlorocyclobutane,
C₄Cl₈ and Further study of the structure of C₈F₁₂.

Owen, Thomas Barron

Purdue University

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THESIS

I. THE STRUCTURE OF
OCTACHLOROCYCLOBUTANE. C_4Cl_8

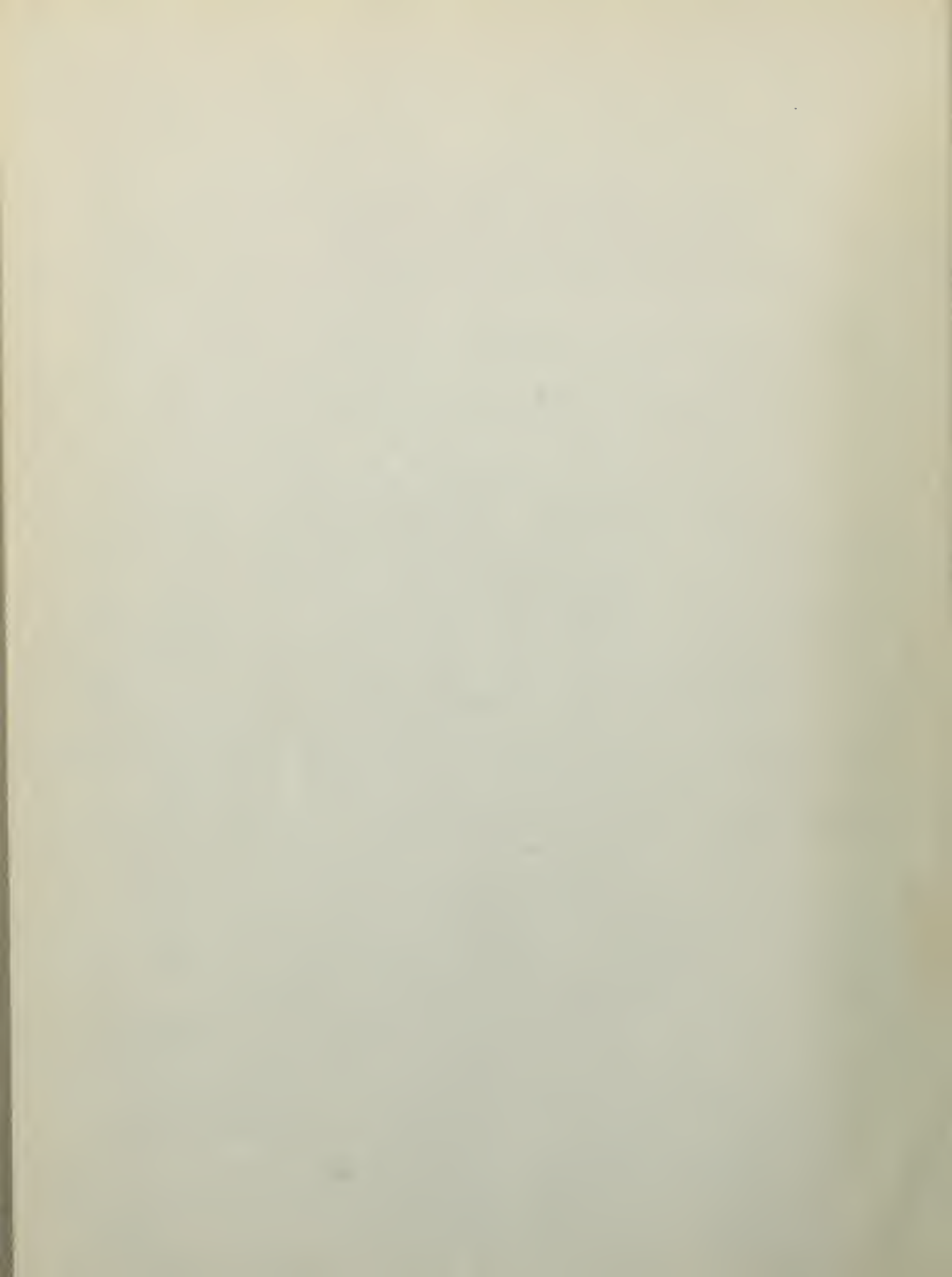
II. FURTHER STUDY OF THE
STRUCTURE OF C_8F_{12}

THOMAS BARRON OWEN

1950

Thesis
095

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- I THE STRUCTURE OF OCTACHLOROCYCLOBUTANE , C_4Cl_8
II FURTHER STUDY OF THE STRUCTURE OF C_8F_{12}

A Thesis

Presented to the Faculty of the Graduate School of
Cornell University for the Degree of
Doctor of Philosophy

By

Thomas Barron Owen

June, 1950

Thesis
095

THE EFFECTS OF CRYSTALLINITY ON THE
MECHANICAL PROPERTIES OF POLYETHYLENE

A Thesis
Submitted to the Faculty of the Graduate School of
Cornell University for the Degree of
Doctor of Philosophy

By
THOMAS BARTON DEAN
June, 1960

BIOGRAPHICAL SKETCH

The author was born on March 19, 1920 in Seattle, Washington. He attended the Seattle public schools and was graduated from Broadway High School in 1936. In June, 1940 he received the degree of Bachelor of Science in Chemical Engineering, cum laude. While employed by the Union Oil Company of California, he was called to active duty in the United States Navy in December of that year. After five years overseas service he returned to this country with the permanent rank of Lieutenant Commander, United States Navy. He studied electronic engineering for one year at the United States Naval Postgraduate School, Annapolis, Maryland and then entered Cornell University in 1947.

He was married to Rosemary Stolz in December, 1944 and has two children, Catherine Adams and Thomas Jr. of ages four and two respectively.

The subject was born on March 22, 1920 in Seattle, Washington. He attended the Seattle Public Schools and was graduated from Everett High School in 1938. In 1939, he received the degree of Bachelor of Science in Chemical Engineering, from Idaho. While employed by the Union Oil Company of California, he was called to active duty in the United States Navy in December of that year. After five years overseas service he returned to this country with the permanent rank of Lieutenant Commander, United States Navy. He studied electronic engineering for one year at the United States Naval Postgraduate School, San Diego, California and then entered Cornell University in 1947.

He was married in Rosemary Hills in December, 1944 and has two children, Catherine Adams and Thomas Jr. of ages four and ten respectively.

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He is particularly grateful to Professors J. L. Hoard, P. Morrison, and E. R. Van Artsdalen for their inspiration and guidance during his tour of duty at Cornell University.

In future assignments it is felt that the experience he has gained here will serve to increase the mutual respect and understanding of the scientist and the naval officer.

The author wishes to express his appreciation to
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hospitality and guidance during his year of study at
Cornell University.

In future assignments he is sure that the opportunity
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PART I

THE STRUCTURE OF OCTACHLOROCYCLOBUTANE , C_4Cl_8

THE JOURNAL OF THE AMERICAN MEDICAL ASSOCIATION
PUBLISHED WEEKLY
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Vol. 13, No. 19

INTRODUCTION

During the past few years Professor W. T. Miller and his students have been engaged in the preparation and study of a variety of fluoro- and chlorocarbons. One of the most interesting of these is the saturated dimer of hexafluorobutadiene, $C_8 F_{12}$,^(1e) the structure of which is to be discussed in part II of this thesis. X-ray studies of this compound thus far have been predicated on a molecular model possessing a center of symmetry which, if it were to exist, would greatly simplify the structure problem. Since $C_8 F_{12}$ is thought to contain three fused cyclobutane rings it would be desirable to know whether or not a simple cyclobutane structure has a plane or puckered ring. If puckering of the ring were confirmed, it would be reasonable to assume that the molecule of $C_8 F_{12}$ has no center of symmetry.

In reviewing the literature it is found that spectroscopic studies of cyclobutane and of its fluorinated analogue $C_4 F_8$ have been interpreted as indicating the carbon ring to be planar. Dunitz⁽⁸⁾ in the X-ray study of one form of tetraphenyl cyclobutane found the structure to have a planar ring also. He states however that an isomer of this compound may have a fourfold alternating axis of symmetry (S_4). However Livingston⁽¹⁴⁾

During the past few years Professor W. F. Miller and his students have been engaged in the investigation and study of a variety of (1) and (2) chlorophylls. One of the most interesting of these is the chlorophyll (3) of *Peridinium*, (4) which is in the chloroplast in part 11 of this book. Other studies of this compound show that it has been previously called in a material which possesses a center of symmetry. It is now in part, which is slightly different from the previous product. When C_{2v} is thought in connection with these chlorophylls it would be desirable to know whether or not a single chlorophyll structure has a plane of symmetry. It is possible that the chlorophylls were combined. It would be desirable to know that the molecule of C_{2v} has an order of symmetry. In studying the literature it is found that specific studies of chlorophylls and of the chlorophylls (5) have been reported as indicating the same type of structure. (6) In the 1935 study of one form of chlorophyll (7) it was found that there are also a chlorophyll ring also. The chlorophyll (8) as shown in this diagram may have a chlorophyll ring- (9) using axis of symmetry (10). (11) However, (12)

in a private communication to this Department has stated that preliminary evidence from the electron diffraction investigation of C_4F_8 indicates a puckered ring with unusually long carbon - carbon distances.

Recently Mr. Fred McLafferty working under Professor Miller's direction has prepared octochlorocyclobutane, C_4Cl_8 , thus making it available for X-ray studies. This presented an excellent opportunity to establish the configuration of the four-membered carbon ring so as to obtain ideas of the probable structure of C_8F_{12} .

Part I of this dissertation concerns itself with the investigation of the structure of C_4Cl_8 .

[illegible]

EXPERIMENTAL PROCEDURE

Preparation and Mounting of Samples.

As remarked above, the compound was prepared by Mr. Fred McLafferty. Essentially the synthesis consists of chlorinating butadiene to give a chlorobutene which in the presence of $AlCl_3$ at $100^\circ C.$ gives several products, one of which is C_4Cl_3 . The material is separated and purified by recrystallization from methyl alcohol.

A portion of the sample was dissolved in benzene in a small test tube and allowed to crystallize slowly overnight. Clear flat needle-like crystals were obtained which when examined microscopically between crossed Nicol prisms showed continuous extinction parallel to the needle axis irrespective of any angular rotation about this axis. Nevertheless, it later appeared that the needle axis was not the unique symmetry axis of the monoclinic crystal.

A needle approximately 0.3 mm. in diameter was mounted vertically on the goniometer head such that the needle axis coincided with the rotation axis. Since the compound has an appreciable vapor pressure it was necessary to dip the crystal in a solution of Canada balsam in xylene to form a protective coating which

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A portion of the sample was dissolved in benzene
in a small test tube and allowed to crystallize slowly
overnight. Clear flat needle-like crystals were obtained
which when examined microscopically between crossed
polarizers showed continuous extinction parallel to
the needle axis irrespective of any regular rotation
about this axis. Invertin, if later specimens that
the crystals are not the same symmetry axis of the
molecular repeat.

A needle approximately 0.1 mm. in diameter was
mounted vertically on the polarimeter head with fast
the needle axis coincided with the rotation axis. Since
the compound was an optically active substance it was
necessary to tilt the crystal in a position of constant
rotation in order to have a positive rotation which

would prevent sublimation. Prior to photography coarse adjustments for alignment were made on a one circle goniometer.

Photographic Recording of Diffraction Data.

Oscillation photographs were taken and the method of Hendershot⁽¹²⁾ was employed to align the crystal for use on the Weissenberg instrument. The oscillation pictures indicated a spacing of 0.3 \AA along the needle axis which was tentatively designated as the c axis.

The zero and four higher layer equi-inclination Weissenberg photographs of this crystal were obtained using $\text{Cu K}\alpha$ radiation. The observed symmetry of the X-ray diffraction effects was $C_{2h} - 2/m$ with the monoclinic axis lying in a plane normal to the needle axis. Only $(0k0)$ reflections for k odd were missing. The following space groups satisfy these conditions: $C_2^2 - P2_1$ or $C_{2h}^2 - P2_1/m$. The latter has a center of symmetry, whereas the former does not.

To obtain sufficient data for structure analysis it is necessary to observe reflections for rotation about at least one other axis. Since the unit cell is monoclinic, the unique axis which lies in the cross section of the needle-like crystals could be located. Sections perpendicular to the needle axis were cut out

using a sharp razor blade. The approximate orientation of the monoclinic axis was known from a comparison of the symmetry of the reflections obtained on the original oscillation photographs with the crystal position. Again oscillation pictures were used for alignment and the zero and six upper layer equi-inclination Weissenberg photographs were obtained for rotation about the monoclinic axis, b. The triple film technique was used throughout.

Lattice Constants.

The lattice constants were determined from the two zero layer Weissenberg photographs (i.e. around b and c) upon which reflections from NaCl had been superimposed. The monoclinic angle was determined by the method of angular lag as described by Buerger⁽⁵⁾ and by direct measurement on the zero layer b-axis film. Final values are:

$$\underline{a} = 8.00 \text{ \AA.}$$

$$\underline{b} = 10.64$$

$$\underline{c} = 6.28$$

$$\beta = 107^{\circ}45'$$

Molecules per Unit Cell.

Although no pycnometric density has been measured for this compound, it was reasonable to assume it roughly

as 2 gm./cc. The volume of the unit cell is 509.5 \AA^3 .

Thus from the formula

$$= 1.660 \text{ nM/V}$$

where n = number of molecules per unit cell

M = molecular weight

V = volume of unit cell in \AA^3

we get, for $n=2$, an X-ray density of 2.16 gm./cc.

Measurement of Intensities.

The reflections were indexed and the value of $\sin \theta$ for each spot was determined graphically from construction of the reciprocal lattice. The method is described by Bunn.⁽⁶⁾ Relative intensities for each film of each layer photograph were estimated by visual comparison with a calibrated intensity scale having spots of a size comparable to those appearing on the films and with the following range of intensities:

2:3:5:6:9:11:13:15:19:22:26:30:35:40:42:43:50:57:64:76:
79:82:88:100:118:130:139:145:147.

The value of 2 indicated a spot that was just visible whereas that of 147 indicated near saturation. The use of the triple film technique permitted a good estimation of intensities over a wide range. The values obtained were corrected for the Lorentz and Polarization factor and the Tunell⁽¹⁹⁾ factor where applicable to obtain relative $|F_{hkl}|^2$ values.

relative values. $\frac{1}{\lambda_{\text{rel}}}$

The zero layer Weissenberg photograph about c was taken as the standard film and by careful cross-calibration all relative $|F_{hk\ell}|^2$ were reduced to the common level. The factors by which the observations from the respective films were multiplied to reach the common level are listed below:

c_1	1.18	b_0	4.15
c_2	1.23	b_1	1.52
c_3	1.82	b_2	1.54
c_4	2.86	b_3	1.25
		b_4	0.95
		b_5	1.43
		b_6	1.43

where the letter denotes the axis of rotation and the subscript the layer line.

The effects of absorption were small enough to be neglected.

DETERMINATION OF ATOMIC POSITIONS

All summations described here were calculated using Beever's and Lipson⁽²⁾ strips.

Patterson Projection, $P(X,Y)$.

Since $hk0$ data were first available the Patterson projection, $P(X,Y)$ on the (001) plane was made.

For the diffraction symmetry for this crystal

$$|F_{hk0}|^2 = |F_{\bar{h}k0}|^2 = |F_{h\bar{k}0}|^2 = |F_{\bar{h}\bar{k}0}|^2;$$

and it can be shown that

$$\begin{aligned} P(X,Y) = & 4 \sum_{h=1}^{\infty} \sum_{k=1}^{\infty} |F_{hk0}|^2 \cos 2\pi hX \cos 2\pi kY \\ & + 2 \sum_{h=1}^{\infty} |F_{h00}|^2 \cos 2\pi hX \\ & + 2 \sum_{k=1}^{\infty} |F_{0k0}|^2 \cos 2\pi kY + |F_{000}|^2. \end{aligned}$$

This projection was used to determine with which of the two space groups, $P2_1$ or $P2_1/m$, the data were consistent. If the former is correct, $P(X,Y)$ should have peaks at $(2x, 1/2)$ for each pair of equivalent atoms in the cell as well as peaks due to vectors between non-equivalent atoms.

If the space group $P2_1/m$ is correct, atoms lying in the planes of symmetry occupy positions:

(e) $x, 1/4, z; \bar{x} 3/4, \bar{z}$. For atoms in fourfold positions there are the following positions:

All elements defined here were obtained using
 Gauss and Legendre's method.

Let \mathcal{H} be the Hilbert space

then the norm $\| \cdot \|$ on \mathcal{H} is defined by the expression
 $\| f \|^2 = \int_0^1 |f(x)|^2 dx$ on the interval $[0, 1]$ where f is real.

For the orthogonal expansion for this space

$$f(x) = \sum_{n=0}^{\infty} a_n \phi_n(x) \quad \text{with} \quad \int_0^1 \phi_n(x) \phi_m(x) dx = \delta_{nm}$$

and it can be shown that

$$\| f \|^2 = \sum_{n=0}^{\infty} |a_n|^2 \quad \text{and} \quad \int_0^1 |f(x)|^2 dx = \sum_{n=0}^{\infty} |a_n|^2$$

$$a_n = \int_0^1 f(x) \phi_n(x) dx$$

$$a_n = \int_0^1 f(x) \phi_n(x) dx$$

This projection was used to determine the value

of the space group \mathcal{H} at \mathcal{H}^* and the value

consequently. If the value is small, \mathcal{H}^* would

have been as large as \mathcal{H} for some value of \mathcal{H}^* and

in the case of well as \mathcal{H} and in some cases \mathcal{H}^*

equivalent values.

If the space group \mathcal{H}^* is small, then \mathcal{H} is

in the plane of symmetry group \mathcal{H}^* .

Let \mathcal{H}^* be the space group. For some \mathcal{H}^* the value is

the following conditions:

(f) $x, y, z; \bar{x}, \bar{y}, \bar{z}; x, 1/2 - y, z; \bar{x}, y + 1/2, \bar{z}$. Vectors between equivalent atoms occupying twofold positions will give rise to peaks at $(2x, 1/2)$ whereas those between equivalent atoms occupying fourfold positions will give rise to peaks at:

$$\begin{aligned} &2\bar{x}, 2\bar{y}; 0, 1/2 - 2y; 2\bar{x}, 1/2; 2x, 1/2; 0, 2y + 1/2; 2\bar{x}, 2y; \\ &2x, 2y; 0, 2y - 1/2; 2x, -1/2; 2\bar{x}, -1/2; 0, -2y - 1/2; 2x, 2\bar{y}. \end{aligned}$$

The projection is shown in Figure 1. Only one-fourth the plane is shown since the other quarters are related to the first by two mutually perpendicular mirror planes as can be seen from a consideration of the Patterson function.

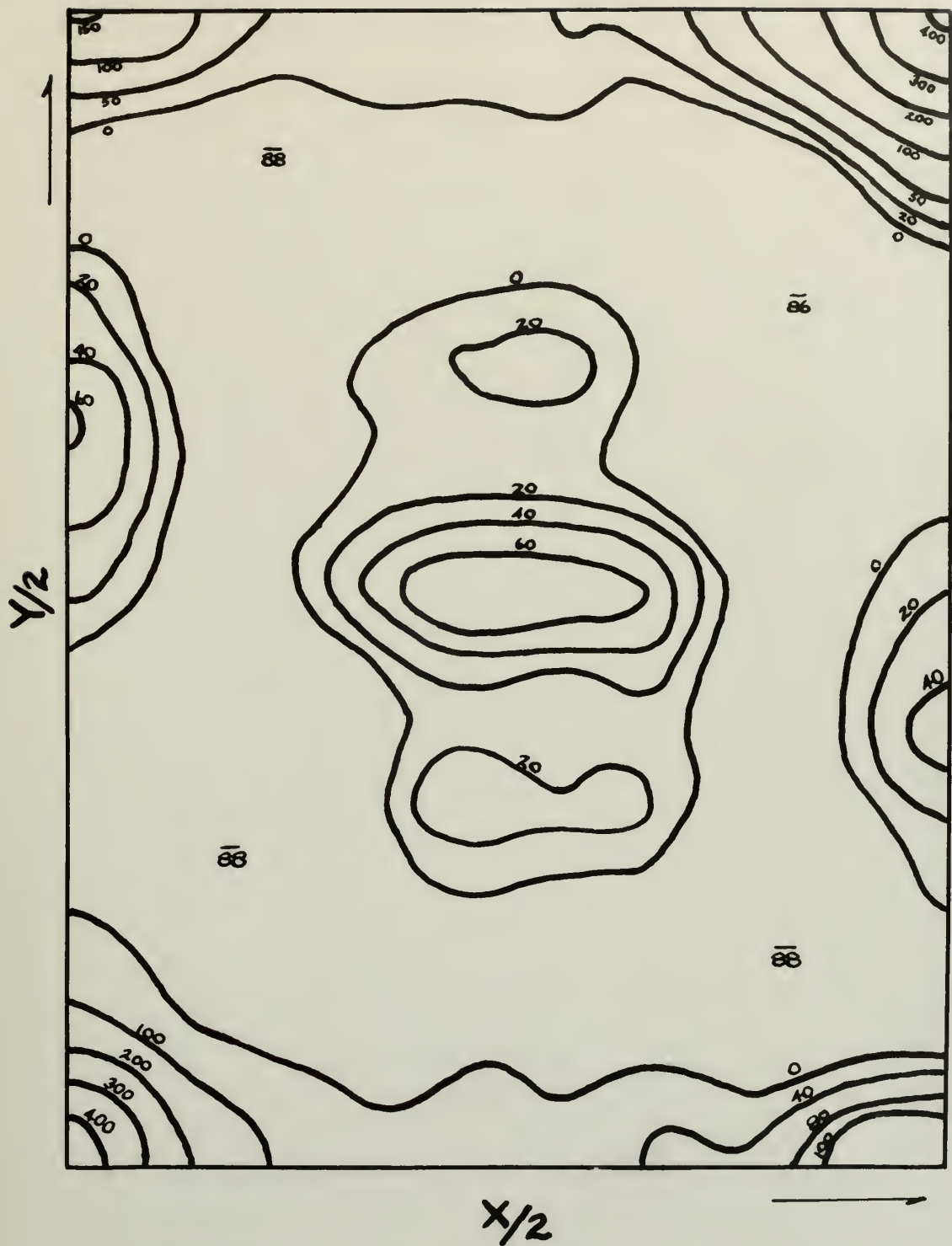
If the centrosymmetrical group be correct and if one considers the orientation of a model of the molecule with respect to the symmetry plane, he should be able to predict the positions of compatible peaks in the Patterson. If the ring lay in the plane one would expect a strong Cl-Cl peak at $X=0, Y=0.3$ but such an orientation would give no peak at $X=0, Y=0.5$. If no atoms lay in the symmetry plane the molecule would have to be oriented such that the symmetry plane bisected the parallel legs of the carbon ring. Again one would expect a strong Cl-Cl peak along $X=0$ but not at $X=0, Y=1/2$. The last possibility is that the diagonal of the carbon ring could lie in the symmetry plane.

[illegible]

location.

It is also noted that the location is shown in Figure 1. Only one-

22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, 160, 161, 162, 163, 164, 165, 166, 167, 168, 169, 170, 171, 172, 173, 174, 175, 176, 177, 178, 179, 180, 181, 182, 183, 184, 185, 186, 187, 188, 189, 190, 191, 192, 193, 194, 195, 196, 197, 198, 199, 200, 201, 202, 203, 204, 205, 206, 207, 208, 209, 210, 211, 212, 213, 214, 215, 216, 217, 218, 219, 220, 221, 222, 223, 224, 225, 226, 227, 228, 229, 230, 231, 232, 233, 234, 235, 236, 237, 238, 239, 240, 241, 242, 243, 244, 245, 246, 247, 248, 249, 250, 251, 252, 253, 254, 255, 256, 257, 258, 259, 260, 261, 262, 263, 264, 265, 266, 267, 268, 269, 270, 271, 272, 273, 274, 275, 276, 277, 278, 279, 280, 281, 282, 283, 284, 285, 286, 287, 288, 289, 290, 291, 292, 293, 294, 295, 296, 297, 298, 299, 300, 301, 302, 303, 304, 305, 306, 307, 308, 309, 310, 311, 312, 313, 314, 315, 316, 317, 318, 319, 320, 321, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 336, 337, 338, 339, 340, 341, 342, 343, 344, 345, 346, 347, 348, 349, 350, 351, 352, 353, 354, 355, 356, 357, 358, 359, 360, 361, 362, 363, 364, 365, 366, 367, 368, 369, 370, 371, 372, 373, 374, 375, 376, 377, 378, 379, 380, 381, 382, 383, 384, 385, 386, 387, 388, 389, 390, 391, 392, 393, 394, 395, 396, 397, 398, 399, 400, 401, 402, 403, 404, 405, 406, 407, 408, 409, 410, 411, 412, 413, 414, 415, 416, 417, 418, 419, 420, 421, 422, 423, 424, 425, 426, 427, 428, 429, 430, 431, 432, 433, 434, 435, 436, 437, 438, 439, 440, 441, 442, 443, 444, 445, 446, 447, 448, 449, 450, 451, 452, 453, 454, 455, 456, 457, 458, 459, 460, 461, 462, 463, 464, 465, 466, 467, 468, 469, 470, 471, 472, 473, 474, 475, 476, 477, 478, 479, 480, 481, 482, 483, 484, 485, 486, 487, 488, 489, 490, 491, 492, 493, 494, 495, 496, 497, 498, 499, 500, 501, 502, 503, 504, 505, 506, 507, 508, 509, 510, 511, 512, 513, 514, 515, 516, 517, 518, 519, 520, 521, 522, 523, 524, 525, 526, 527, 528, 529, 530, 531, 532, 533, 534, 535, 536, 537, 538, 539, 540, 541, 542, 543, 544, 545, 546, 547, 548, 549, 550, 551, 552, 553, 554, 555, 556, 557, 558, 559, 560, 561, 562, 563, 564, 565, 566, 567, 568, 569, 570, 571, 572, 573, 574, 575, 576, 577, 578, 579, 580, 581, 582, 583, 584, 585, 586, 587, 588, 589, 590, 591, 592, 593, 594, 595, 596, 597, 598, 599, 600, 601, 602, 603, 604, 605, 606, 607, 608, 609, 610, 611, 612, 613, 614, 615, 616, 617, 618, 619, 620, 621, 622, 623, 624, 625, 626, 627, 628, 629, 630, 631, 632, 633, 634, 635, 636, 637, 638, 639, 640, 641, 642, 643, 644, 645, 646, 647, 648, 649, 650, 651, 652, 653, 654, 655, 656, 657, 658, 659, 660, 661, 662, 663, 664, 665, 666, 667, 668, 669, 670, 671, 672, 673, 674, 675, 676, 677, 678, 679, 680, 681, 682, 683, 684, 685, 686, 687, 688, 689, 690, 691, 692, 693, 694, 695, 696, 697, 698, 699, 700, 701, 702, 703, 704, 705, 706, 707, 708, 709, 710, 711, 712, 713, 714, 715, 716, 717, 718, 719, 720, 721, 722, 723, 724, 725, 726, 727, 728, 729, 730, 731, 732, 733, 734, 735, 736, 737, 738, 739, 740, 741, 742, 743, 744, 745, 746, 747, 748, 749, 750, 751, 752, 753, 754, 755, 756, 757, 758, 759, 760, 761, 762, 763, 764, 765, 766, 767, 768, 769, 770, 771, 772, 773, 774, 775, 776, 777, 778, 779, 780, 781, 782, 783, 784, 785, 786, 787, 788, 789, 790, 791, 792, 793, 794, 795, 796, 797, 798, 799, 800, 801, 802, 803, 804, 805, 806, 807, 808, 809, 810, 811, 812, 813, 814, 815, 816, 817, 818, 819, 820, 821, 822, 823, 824, 825, 826, 827, 828, 829, 830, 831, 832, 833, 834, 835, 836, 837, 838, 839, 840, 841, 842, 843, 844, 845, 846, 847, 848, 849, 850,



PATTERSON PROJECTION

$P(XY)$

Figure 1

If a scaled molecular model is so oriented and allowed to pucker it can be seen that the last configuration would give rise to two different Cl-Cl separations parallel to the unique axis. The shorter Cl-Cl vector would cause a peak at $X=0$ somewhere between $Y=1/4$ and $Y=1/2$. The longer vector would show up at $X=0$ and near $Y=1/2$. Such maxima do appear in the projection so this orientation of the molecule is consistent thus far. The peak at $X=1/2$, $Y=0.19$ if caused by a set of equivalent fourfold atoms would also mean a peak at $X=0$ $y=0.31$ (i.e. $2x=1/2$, $2y=0.19$ corresponds to $0, 0.50-0.19$ or $0, 0.31$) if one considers the list above. Also, if the peak at $X=1/2$, $Y=1/2$ included a vector due to the other set of fourfold chlorines one would expect a peak at $X=0$, $Y=1/2$ which indeed is obtained. The chosen position of the molecule thus fits in with the interpretation of the Patterson and all peaks can be explained. The projection is then consistent with the space group, $P2_1/m$.

It was possible to assign x and y parameters to the chlorine atoms of the molecule and by assuming normal C-C bond lengths to assign parameters to the carbons as well. These were:

x	y	x	y	x	y
C_1 +0.125	$1/4$	Cl_1 +0.235	+0.092	Cl_6 +0.045	$1/4$
C_2 +0.250	+0.156	Cl_4 +0.255	+0.255	Cl_7 -0.075	$1/4$
C_3 +0.375	$1/4$	Cl_5 +0.465	$1/4$	Cl_8 +0.565	$1/4$

It is claimed molecular model is an unphysical one

allowed to predict it can be seen that the last configuration

tion would give rise to the different C_1-C_2 separation

parallel to the carbon axis. The distance C_1-C_2 would

smaller than a peak at low temperature between $2\pi/\lambda$ and

$2\pi/\lambda$. The longer vector would show up at low and high

$2\pi/\lambda$. When making the approximation in the projection of this

extension of the molecule is consistent with this. The

peak at $2\pi/\lambda$, $2\pi/\lambda$ is caused by a set of configurations

characteristic of the molecule with a peak at $2\pi/\lambda$.

(i.e. $2\pi/\lambda$, $2\pi/\lambda$ is characteristic of $0.05-0.10$ or 0.11)

It now characterizes the first vector. Also, it has peak at

$2\pi/\lambda$, $2\pi/\lambda$ for which a vector due to the other set of

configurations would expect a peak at $2\pi/\lambda$, $2\pi/\lambda$

which indeed is obtained. The chosen position at the

molecule thus fits in with the interpretation of the

extension and all peaks can be explained. The projection

is then consistent with the given group, $2\pi/\lambda$.

It was possible to assign a and y parameters to the

relative areas of the molecule and by assuming normal

C_1-C_2 bond lengths to assign parameters to the carbon

as well. These were:

x	y	z	x	y	z
$C_1 + 0.125$	$1/2$	$0.125 + 0.125$	0.125	0.125	0.125
$C_2 + 0.125$	0.125	$0.125 + 0.125$	0.125	0.125	0.125
$C_3 + 0.125$	$1/2$	$0.125 + 0.125$	0.125	0.125	0.125

It might be well to describe the configuration of the molecule as postulated. In the symmetry plane the four chlorines form an isosceles trapezoid. The perpendicular bisector of the bases of this quadrilateral lies almost along the trace of the plane $x=1/4$ in the symmetry plane. The four chlorine atoms out of the plane also form a trapezoid the plane of which is almost coincident with $x=1/4$. Figure 2 is a sketch of the molecule and will serve to clarify the above. The puckering of the ring can be seen.

Amplitude Calculations.

For the space group $P2_1/m$ it can be shown that the contribution to the reflection amplitude $F_{hk\ell}$ from two like atoms occupying twofold positions is

$$\begin{aligned} A &= 2fa \cos 2\pi(hx + \ell z) \cos \frac{\pi k}{2} \text{ for } k \text{ even} \\ &= -2fa \sin 2\pi(hx + \ell z) \sin \frac{\pi k}{2} \text{ for } k \text{ odd} \end{aligned}$$

where fa is the atomic scattering power of the atom. The contribution from four like atoms occupying fourfold positions is

$$\begin{aligned} A &= 4fa \cos 2\pi(hx + \ell z) \cos 2\pi ky \text{ for } k \text{ even} \\ \text{and } A &= -4fa \sin 2\pi(hx + \ell z) \sin 2\pi ky \text{ for } k \text{ odd.} \end{aligned}$$

From these relations the following relations can be deduced:

$$\begin{aligned} F_{hk\ell} &= F_{\overline{h}\overline{k}\overline{\ell}} \text{ for all } k \\ F_{hk\ell} &= F_{h\overline{k}\ell} \text{ for } k \text{ even} \\ F_{hk\ell} &= -F_{h\overline{k}\ell} \text{ for } k \text{ odd.} \end{aligned}$$

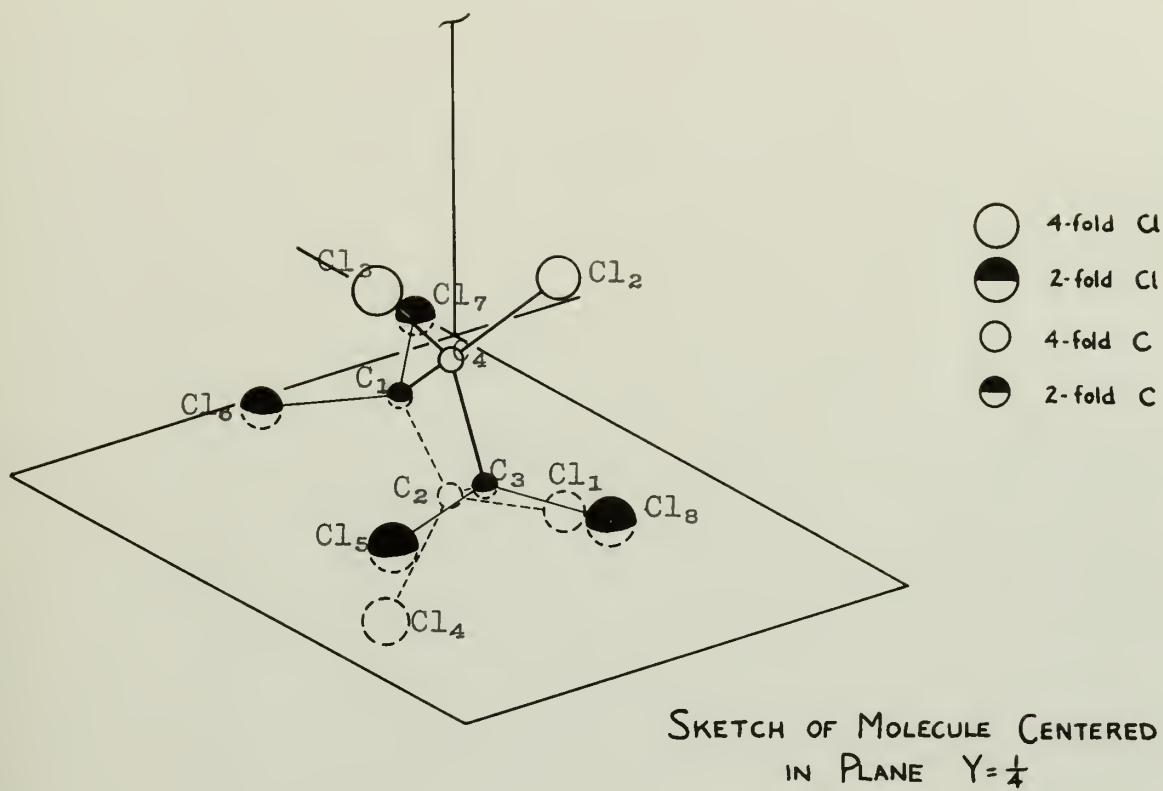
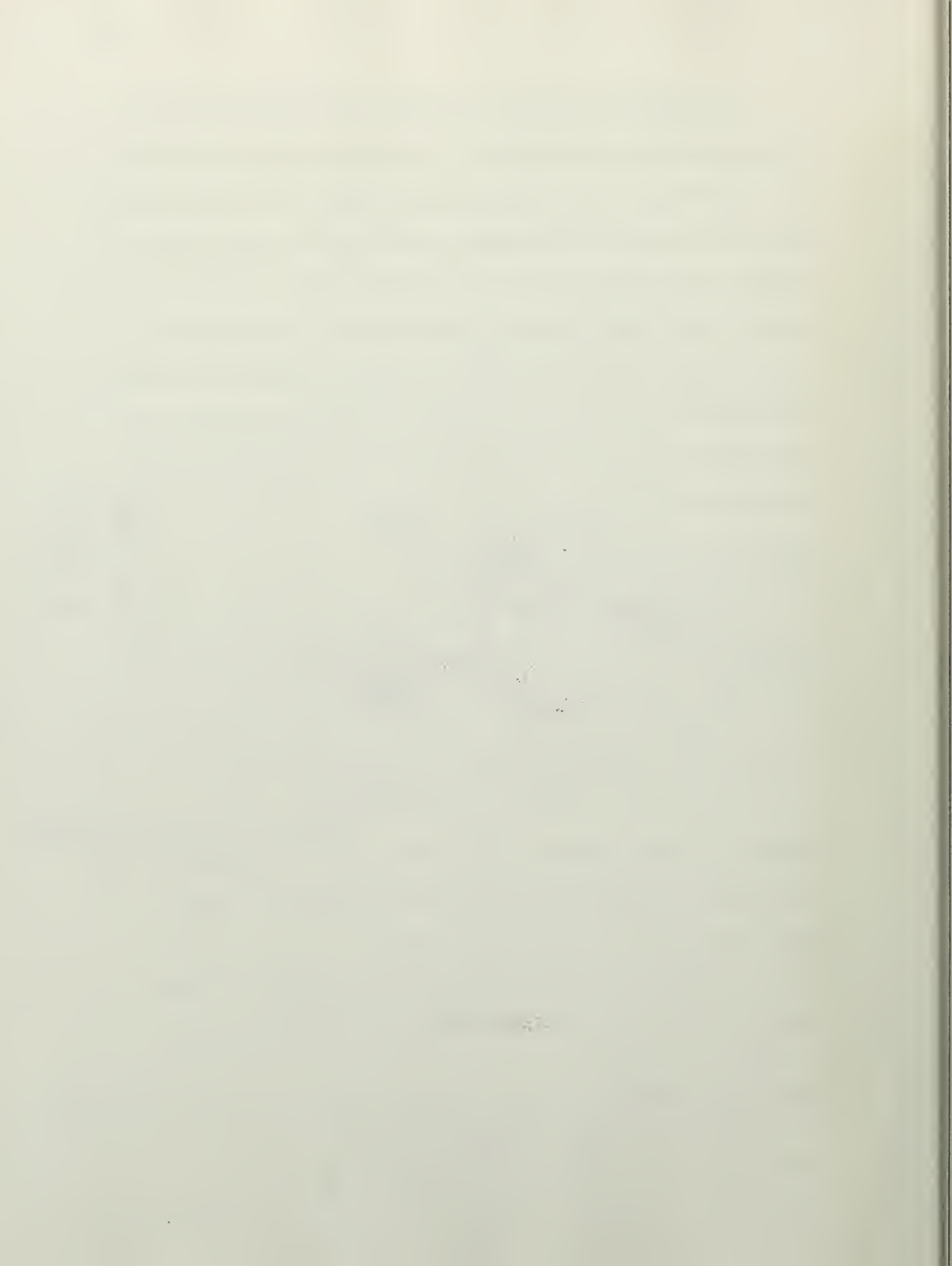


Figure 2



Fourier Projection, $\rho(x,y)$.

Using the trial parameters obtained from the interpretation of the Patterson, the phases for (hk0) data were calculated in order to make the Fourier projection, $\rho(x,y)$, on (001). It can be shown that

$$\begin{aligned} K \rho(x,y) = & 4 \sum_{h=1}^{\infty} \sum_{\substack{k=2n \\ n \geq 1}}^{\infty} F_{hk0} \cos 2\pi hx \cos 2\pi ky \\ & + 2 \sum_{h=1}^{\infty} F_{h00} \cos 2\pi hx + 2 \sum_{\substack{k=2n \\ n \geq 1}}^{\infty} F_{0k0} \cos 2\pi ky \\ & - 4 \sum_{h=1}^{\infty} \sum_{\substack{k=2n+1 \\ n \geq 0}}^{\infty} F_{hk0} \sin 2\pi hx \sin 2\pi ky \end{aligned}$$

(neglecting constant additive terms).

The projection is shown in figure 3. The positions of maxima were not too well resolved, but sufficiently so to confirm the postulated model. Chlorine peaks superimpose to some extent but are clear enough to obtain parameters. Carbon peaks are lost in those of the chlorines so carbon positions must be assigned from consideration of known C-C and C-Cl bond lengths. Atomic coordinates now became:

x	y	x	y	x	y
C ₁ +0.100	1/4	Cl ₁ +0.238	+0.095	Cl ₆ +0.038	1/4
C ₂ +0.234	+0.159	Cl ₄ +0.245	+0.020	Cl ₇ -0.080	1/4
C ₃ +0.383	1/4	Cl ₅ +0.470	1/4	Cl ₈ +0.568	1/4

Fourier projection, $\rho(x, y)$.

Using the trial parameters obtained from the inter-

pretation of the Patterson, the phases for (hkl) data were calculated in order to make the Fourier projection.

$\rho(x, y)$ in (GDI). It can be shown that

$$\rho(x, y) = \frac{1}{V} \sum_{h=1}^N \sum_{k=1}^N \sum_{l=1}^N \cos 2\pi(hx + ky + lz) \rho(h, k, l)$$

$$+ \frac{1}{V} \sum_{h=1}^N \sum_{k=1}^N \sum_{l=1}^N \cos 2\pi(hx + ky + lz) \rho(h, k, l)$$

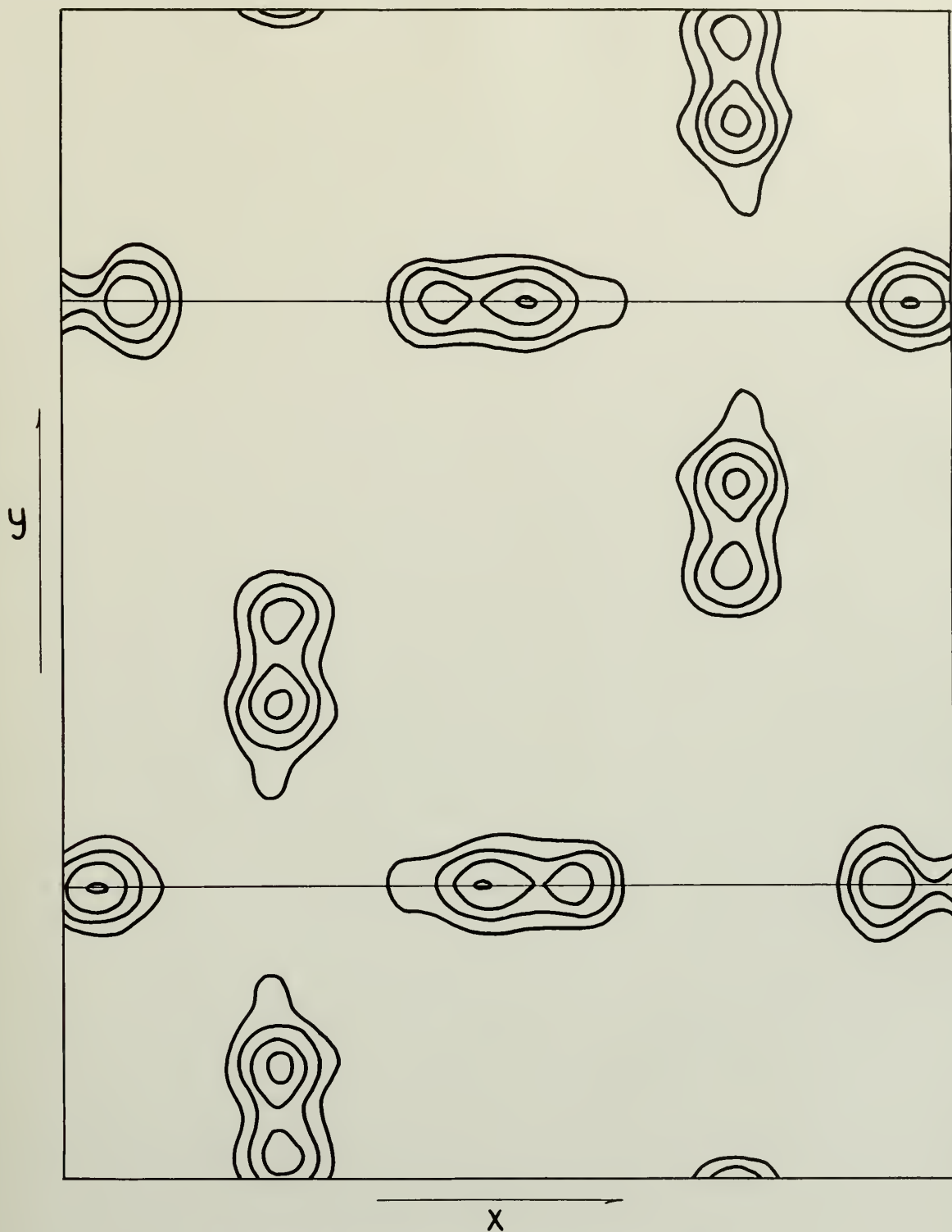
$$- \frac{1}{V} \sum_{h=1}^N \sum_{k=1}^N \sum_{l=1}^N \cos 2\pi(hx + ky + lz) \rho(h, k, l)$$

(neglecting constant additive terms).

The projection is shown in Figure 2. The positions of maxima were not too well resolved, but sufficiently so to confirm the postulated model. Chlorine peaks appear to some extent but are clear enough to obtain preliminary. Carbon peaks are lost in those of the chlorines as carbon positions must be assigned from consideration of known C-C and C-Cl bond lengths. Atomic coordinates

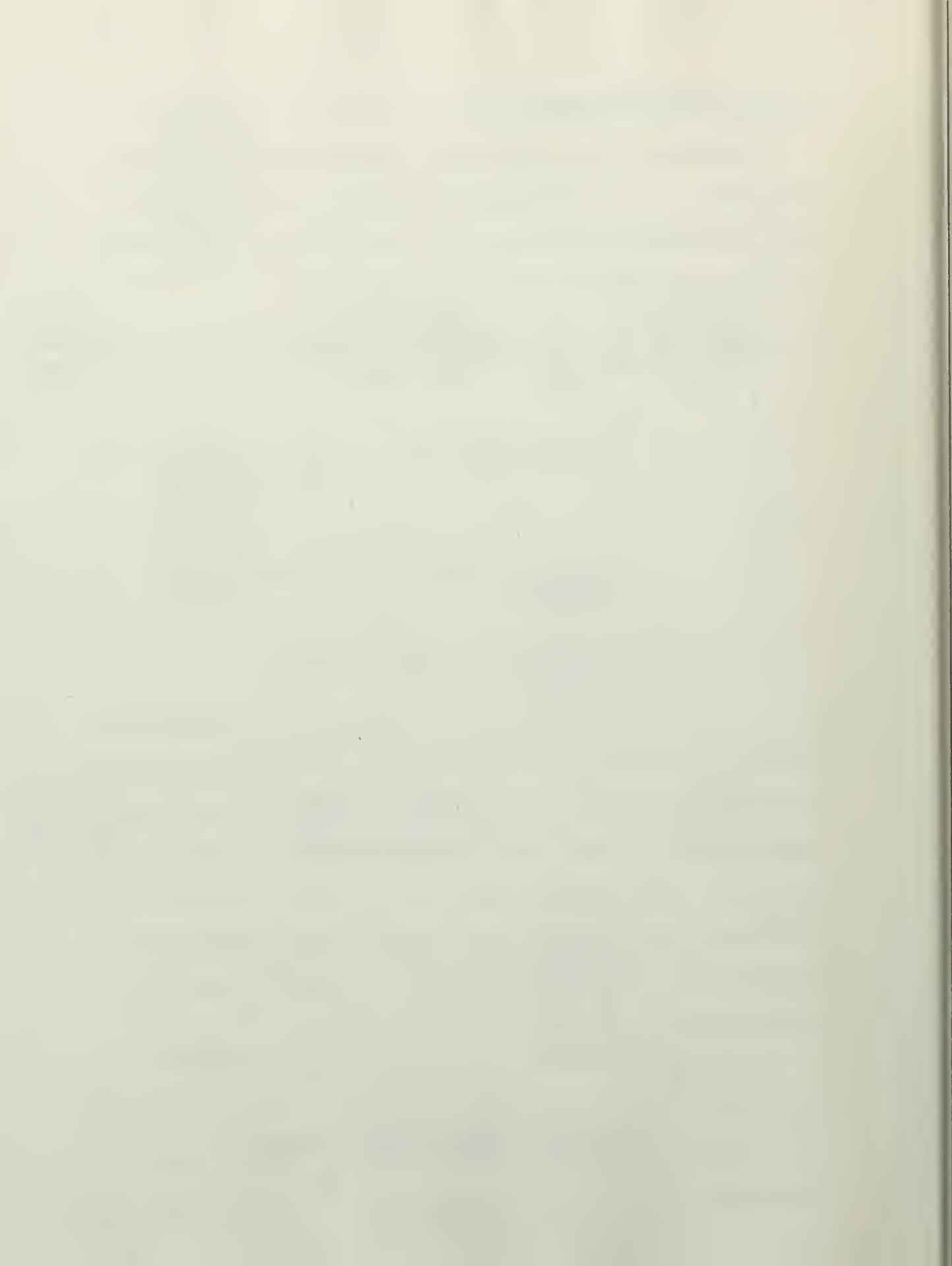
now become:

x	y	x	y	x	y
Cl ¹ +0.100	1/4	Cl ¹ +0.258	+0.092	Cl ¹ +0.258	1/4
Cl ² +0.234	+0.136	Cl ² +0.262	+0.020	Cl ² +0.080	1/4
Cl ³ +0.252	1/4	Cl ³ +0.470	1/4	Cl ³ +0.268	1/4



FOURIER PROJECTION $p(x,y)$

Figure 3



Orientation Along z.

At this stage, x and y coordinates were fairly well determined. The next problem was to determine positions along z. In effect there are two strings of molecules, one centered at $x=1/4, y=1/4$ and the other at $x=3/4, y=3/4$ but the orientation along z of the one string with respect to the other was not yet fixed. Then too there is the question as to the orientation of the trapezoid of the chlorines in the symmetry plane. The projection does not reveal whether the long or short base is most advanced along z.

In an attempt to resolve these ambiguities, reflection amplitudes $F(00\lambda)$ were calculated for motion of the molecule along z with a chosen orientation of the trapezoid. Since no agreement of the calculated amplitudes with those observed was obtained, the obvious step would have been to reverse the molecule and again compare amplitudes.

Patterson Sections $P(0,Y,0)$ and $P(X,1/2,Z)$.

A better idea presented itself however. If one calculates the Patterson section $P(X,1/2,Z)$ he obtains peaks resulting from vectors whose Y separation is $1/2$. For atoms related to each other by the screw axis, peaks should appear in the section at $2x, 1/2, 2z$. Since x parameters are known, one would then be able to determine

Orientation Along z.

At this stage, x and y coordinates were fairly well determined. The next problem was to determine positions along z. In effect there are two strings of molecules, one centered at $x=1/2, y=1/2$ and the other at $x=3/4, y=3/4$ but the orientation along z of the one string with respect to the other was not fixed. Then too there is the question as to the orientation of the triphenyls in the chains in the symmetry plane. The projection does not reveal whether the long or short axis is most advanced along z.

In an attempt to resolve these ambiguities, reflections amplitudes $F(00\lambda)$ were calculated for motion of the molecule along z with a chosen orientation of the triphenyls. Since no agreement of the calculated amplitudes with those observed was obtained, the obvious step would have been to reverse the molecule and again compare amplitudes.

Triphenyl sections $F(0, y, 0)$ and $F(x, 1/2, 1/2)$.

A better idea presented itself however. It was calculated the triphenyl section $F(x, 1/2, 1/2)$ by adding peaks resulting from vectors whose y separation is $1/2$. For atoms related to each other by the screw axis, peaks should appear in the section at $2x, 1/2, 1/2$. Since x parameters are known, one would then be able to determine

z coordinates from peaks that are sufficiently resolved. There will of course be peaks indicating vectors between non-equivalent atoms lying in the symmetry planes.

The sections were made using relative $|F_{hk\ell}|^2$ values divided by an arbitrary temperature factor $e^{-3\left(\frac{\sin\theta}{\lambda}\right)^2}$ to sharpen up the peaks and to improve resolution. At the same time it was decided to compute the Patterson line section $P(0,Y,0)$ which will give peaks corresponding to vectors which are parallel to the unique axis. For the molecule under discussion accurate separations of fourfold chlorine atoms should be observed as indeed they were.

The line section may be expressed as:

$$P(0,Y,0) = |F_{000}|^2 + 2 B_0 + 4 \sum_{k=1}^{\infty} B_k \cos 2 \pi k Y$$

$$\text{where } B_0 = 1/2 \sum_{h=1}^{\infty} |F_{h00}|^2 + 1/2 \sum_{h=-\infty}^{\infty} \sum_{\ell=1}^{\infty} |F_{h0\ell}|^2$$

$$B_k = 1/2 |F_{0k0}|^2 + \sum_{h=1}^{\infty} |F_{hk0}|^2 + \sum_{h=-\infty}^{\infty} \sum_{\ell=1}^{\infty} |F_{hk\ell}|^2$$

Figure 4 shows $P(0,Y,0)$ for C_4Cl_8 . It was only necessary to evaluate the function from $Y=0$ to $Y=1/2$ since the latter point is a center of symmetry.

The peak at $Y=0$ arises from null vectors for each of the atoms in the unit cell. The peak at $Y=0.325$ must be

The first section may be represented as

$$f(x, y, z) = \frac{1}{2\pi} \int_0^{2\pi} \int_0^\pi \frac{1}{\sqrt{1 - k^2 \sin^2 \theta}} \sin \theta d\theta d\phi$$

$$= \frac{1}{2\pi} \int_0^{2\pi} \frac{1}{\sqrt{1 - k^2 \sin^2 \theta}} d\phi$$

$$= \frac{1}{2\pi} \int_0^{2\pi} \frac{1}{\sqrt{1 - k^2 \sin^2 \theta}} d\phi$$

due to the shorter fourfold Cl-Cl spacing in the molecule.
Thus if

$$1/2 - 2y = 0.325$$

$$\text{then } y = 0.083.$$

The peak at $Y=1/2$ is associated with overlapping peaks resulting from the longer fourfold Cl-Cl spacing. If the single peak is resolved into the proper component peaks as shown by the dotted curves in the figure then

$$1/2 - 2y = 0.466$$

$$\text{and } y = 0.017.$$

The small hump at $Y = 0.207$ may be a spurious peak resulting from the "sharpening up" process or may actually correspond to the expected fourfold carbon separation of 2.2 \AA . If

$$1/2 - 2y = 0.206$$

$$\text{then } y = 0.147$$

At any rate, good y parameters may now be assigned to the fourfold chlorines atoms.

Returning to the section $P(X, 1/2, Z)$ it can be shown:

$$\begin{aligned} P(X, 1/2, Z) = & |F_{000}|^2 + 2B_{00} + 4 \sum_{h=1}^{\infty} B_{h0} \cos 2\pi hX \\ & + 4 \sum_{h=0}^{\infty} \sum_{\ell=1}^{\infty} B_{h\ell}^{II} \cos 2\pi hX \cos 2\pi \ell Z \\ & - 4 \sum_{h=0}^{\infty} \sum_{\ell=1}^{\infty} B_{h\ell}^{II} \sin 2\pi hX \sin 2\pi \ell Z \end{aligned}$$

for the vector function $\mathbf{f}(\mathbf{x})$ in the volume.

$$\mathbf{f}(\mathbf{x}) = \mathbf{y} = 0.125$$

$$\mathbf{f}(\mathbf{x}) = \mathbf{y} = 0.125$$

The peak of $\mathbf{f}(\mathbf{x})$ is associated with overlapping peaks resulting from the linear function $\mathbf{f}(\mathbf{x})$ in the volume. It is possible that the linear function $\mathbf{f}(\mathbf{x})$ is not linearly separable from the data points in the volume.

$$\mathbf{f}(\mathbf{x}) = \mathbf{y} = 0.125$$

$$\mathbf{f}(\mathbf{x}) = \mathbf{y} = 0.125$$

The result of $\mathbf{f}(\mathbf{x}) = \mathbf{y} = 0.125$ may be a function of the data points in the volume. It is possible that the linear function $\mathbf{f}(\mathbf{x})$ is not linearly separable from the data points in the volume.

$$\mathbf{f}(\mathbf{x}) = \mathbf{y} = 0.125$$

$$\mathbf{f}(\mathbf{x}) = \mathbf{y} = 0.125$$

At any rate, good $\mathbf{f}(\mathbf{x})$ parameters may now be assigned to the function $\mathbf{f}(\mathbf{x})$.

According to the equation $\mathbf{f}(\mathbf{x}) = \mathbf{y}$, it can be shown:

$$\mathbf{f}(\mathbf{x}) = \mathbf{y} = 0.125$$

$$\mathbf{f}(\mathbf{x}) = \mathbf{y} = 0.125$$

$$\mathbf{f}(\mathbf{x}) = \mathbf{y} = 0.125$$

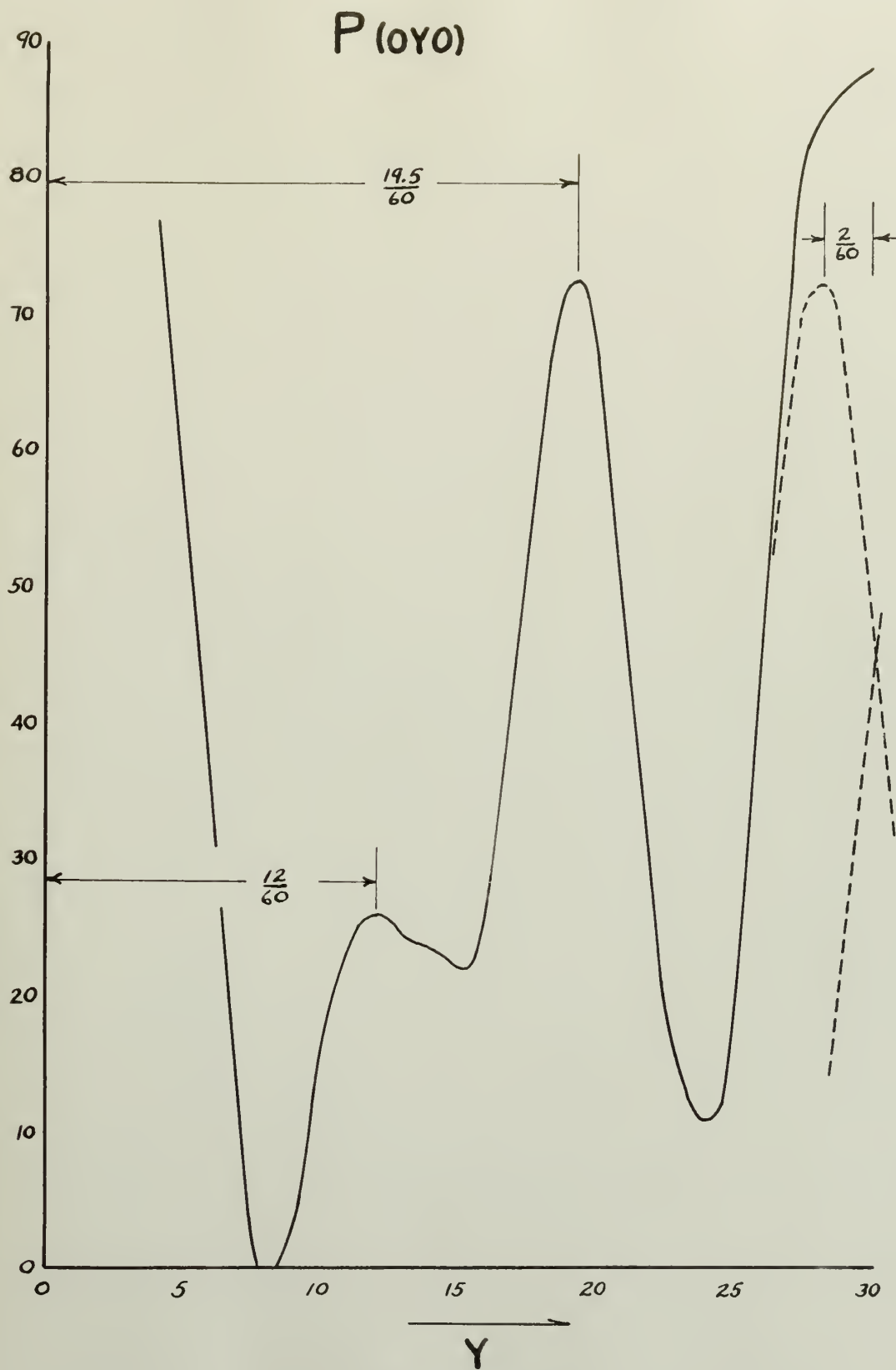


Figure 4

$$\text{where } B_{00} = 1/2 \sum_{k=2}^{\infty} |F_{0k0}|^2$$

$$B_{h0} = 1/2 |F_{h00}|^2 + \sum_{k=1}^{\infty} (-1)^k |F_{hk0}|^2$$

$$B^{1h\ell} = B_{h\ell} + B_{\bar{h}\ell}$$

$$B^{11h\ell} = B_{h\ell} - B_{\bar{h}\ell}$$

$$\text{and } B_{h\ell} = 1/2 |F_{h0\ell}|^2 + \sum_{k=1}^{\infty} (-1)^k |F_{hk\ell}|^2.$$

The section is shown in Figure 5. It is apparent that peaks indicative of vectors of $X = 2x = 1/2$, of which there will be many arising from the fourfold atoms, all run together so cannot be clearly resolved. However by considering the x parameters of the twofold chlorines (i.e. those in the symmetry plane) it was possible to pick the proper orientation of the trapezoid they form and to obtain their proper z coordinates. It was established that the short base of this trapezoid was most advanced in the $+z$ direction and the proper orientation is as shown in Figure 2. Parameter values available now are listed. Small changes in x parameters have occurred as a result of including all the data in the summation.

$$|g_{00}| = \sqrt{2} \sum_{k=1}^{\infty} \frac{1}{k} \quad \text{where}$$

$$g_{00} = \sqrt{2} |f_{00}|^2 + \sum_{k=1}^{\infty} (-1)^k \frac{1}{k} |f_{0k}|^2$$

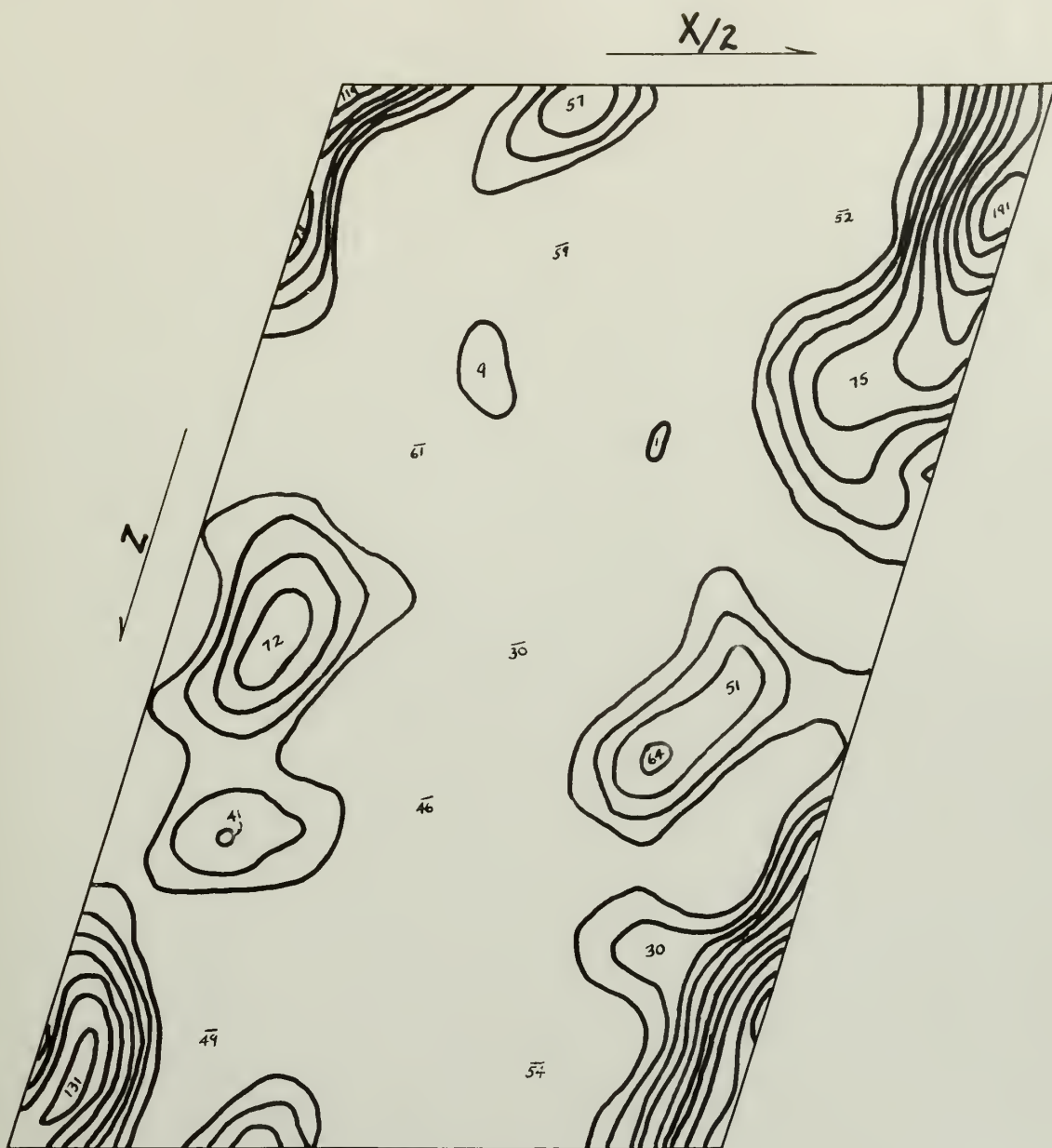
$$g_{11} = g_{22} = g_{33} = 2\pi^2$$

$$g_{12} = g_{13} = g_{23} = 0$$

$$g_{11} = \sqrt{2} |f_{10}|^2 + \sum_{k=1}^{\infty} (-1)^k \frac{1}{k} |f_{1k}|^2 \quad \text{and}$$

The section is shown in Figure 2. It is apparent

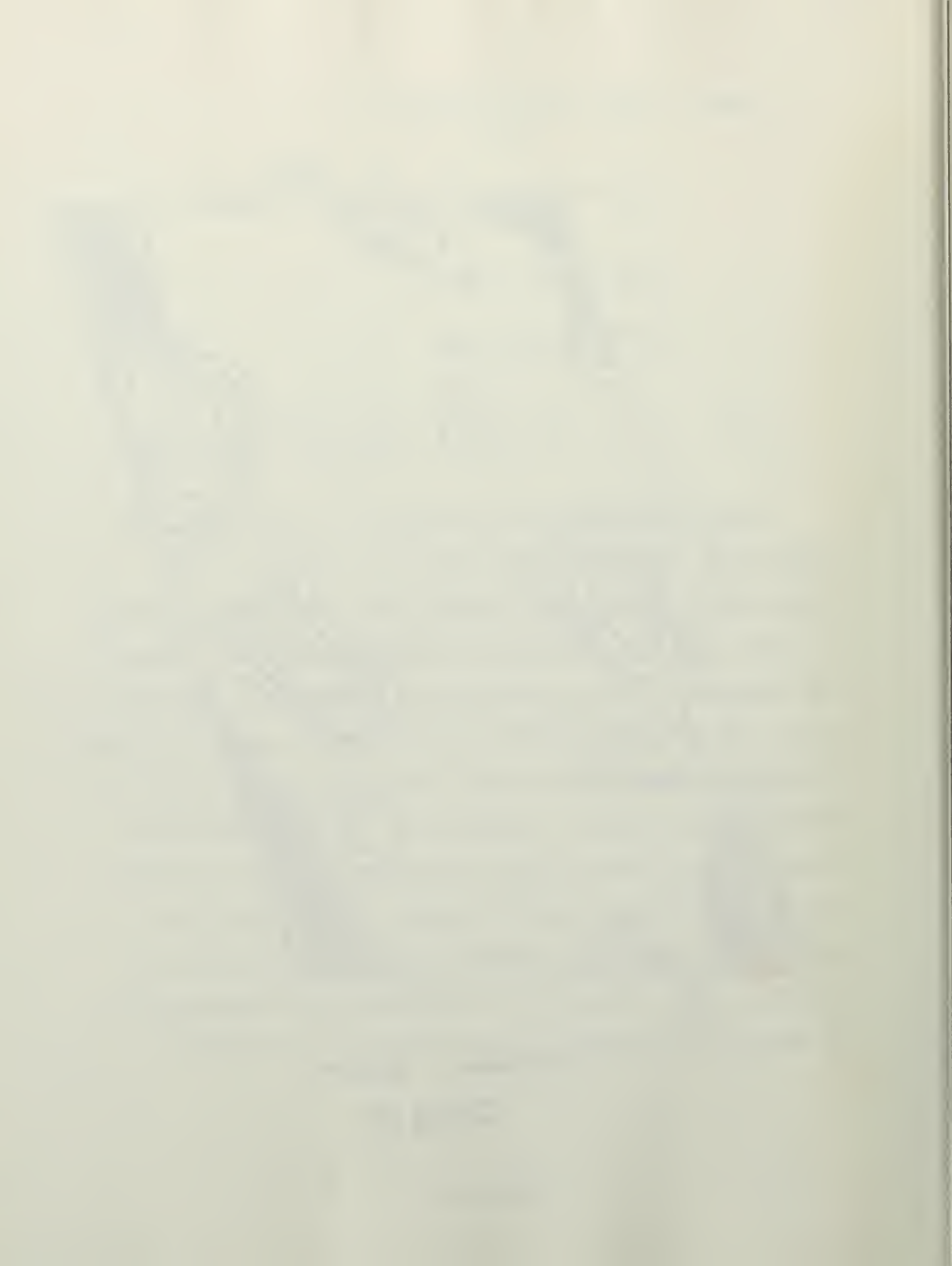
that peaks indicative of vectors of $k = 2\pi/\lambda$ of which there will be many arising from the fourfold axes, all run together so cannot be easily resolved. However by considering the k parameters of the twofold chiralities (i.e. those in the symmetry plane) it was possible to pick the proper orientation of the tripole they form and to obtain their proper k coordinates. It was established that the short case of this tripole was most advanced in the z direction and the proper orientation is as shown in Figure 3. Parameter values available now are listed. Small changes in k parameters have occurred as a result of including all the data in the summation.



PATTERSON SECTION

$$P(x^{\frac{1}{2}}z)$$

Figure 5



	x	y	z
C ₁	+0.108	1/4	+0.238
C ₂	+0.250	+0.147	+0.230
C ₃	+0.392	1/4	+0.362
Cl ₁	+0.245	+0.088	-0.035
Cl ₄	+0.238	+0.017	+0.425
Cl ₅	+0.470	1/4	+0.655
Cl ₆	+0.033	1/4	+0.488
Cl ₇	-0.078	1/4	-0.017
Cl ₈	+0.568	1/4	+0.225

Fourier Projection $\rho(x, z)$.

In order to obtain better x and z coordinates the phases of the $h0\ell$ reflections were calculated and the Fourier projection $\rho(x, z)$ on (010) evaluated. Here

$$\begin{aligned}
 \rho(x, z) = F_{000} + \sum_{h=0}^{\infty} \sum_{\ell=1}^{\infty} (F_{h0\ell} + F_{\bar{h}0\ell}) \cos 2\pi hx \cos 2\pi \ell z \\
 + \sum_{h=1}^{\infty} F_{h00} \cos 2\pi hx \\
 - \sum_{h=1}^{\infty} \sum_{\ell=1}^{\infty} (F_{h0\ell} - F_{\bar{h}0\ell}) \sin 2\pi hx \sin 2\pi \ell z.
 \end{aligned}$$

There was some superposition of peaks corresponding to twofold chlorines in this projection and carbon maxima were rather fuzzy. The fourfold chlorines were well defined. Atomic coordinates were obtained, phases were redetermined,

	x	y	z
C1	+0.108	1/4	+0.123
C2	+0.120	+0.147	+0.130
C3	+0.132	1/4	+0.143
C4	+0.142	+0.158	+0.155
C5	+0.150	+0.167	+0.163
C6	+0.157	1/4	+0.168
C7	+0.163	1/4	+0.173
C8	+0.168	1/4	+0.177
C9	+0.173	1/4	+0.182

Fourier projection $\rho(x, z)$.

In order to obtain better x and z coordinates the phases of the h0k reflections were calculated and the Fourier projection $\rho(x, z)$ on (000) evaluated, where

$$\rho(x, z) = 1000 + \sum_{h=0}^{\infty} \sum_{k=1}^{\infty} (F_{h0k} + F_{\bar{h}0k}) \cos 2\pi h x \cos 2\pi k z$$

$$+ \sum_{h=1}^{\infty} \sum_{k=0}^{\infty} F_{h0k} \cos 2\pi h x$$

$$+ \sum_{h=1}^{\infty} \sum_{k=1}^{\infty} (F_{h0k} - F_{\bar{h}0k}) \sin 2\pi h x \sin 2\pi k z.$$

There was some superposition of peaks corresponding to twofold extinction in this projection and carbon maxima were rather fuzzy. The fourfold extinction were well defined. Atomic coordinates were obtained, phases were redetermined,

and the Fourier function re-evaluated until no sign changes occurred. Figure 6 shows the projection of matter in the unit cell along the unique axis. The overlap of the twofold chlorines is evident. Atomic coordinates are now:

	x	y	z
C ₁	+0.100	1/4	+0.233
C ₂	+0.238	+0.147	+0.262
C ₃	+0.378	1/4	+0.338
Cl ₁	+0.244	+0.088	-0.008
Cl ₄	+0.238	+0.017	+0.423
Cl ₅	+0.467	1/4	+0.636
Cl ₆	+0.012	1/4	+0.458
Cl ₇	-0.092	1/4	-0.003
Cl ₈	+0.572	1/4	+0.255

It may be well to note that coordinates given by the projections $\rho(x,y)$ and $\rho(x,z)$ cannot be considered as final. The X-ray photographs of the crystals show several reflections of considerable amplitude at high values of $(\sin \theta)/\lambda$ indicating that the Fourier series will be slow in converging. To obtain the best set of positions all the data must be used and even then there may be errors due to non-convergence. This point will be discussed later.

and the Fourier transform re-evaluated with no sign changes occurred. Figure 4 shows the projection of the unit cell along the x-axis. The values of the Fourier transform are plotted. Atomic positions are not

x	y	z	f
0.100	0.100	0.100	0.100
0.100	0.100	0.100	0.100
0.100	0.100	0.100	0.100
0.100	0.100	0.100	0.100
0.100	0.100	0.100	0.100
0.100	0.100	0.100	0.100
0.100	0.100	0.100	0.100
0.100	0.100	0.100	0.100
0.100	0.100	0.100	0.100
0.100	0.100	0.100	0.100
0.100	0.100	0.100	0.100
0.100	0.100	0.100	0.100
0.100	0.100	0.100	0.100
0.100	0.100	0.100	0.100
0.100	0.100	0.100	0.100

It may be well to note that coordinates given by the projections $\psi(x,y)$ and $\phi(x,y)$ cannot be considered as final. The 2-ray photographs of the crystals show several reflections of considerable amplitude at high values of ψ and ϕ . Indicating that the Fourier series will be slow in converging. To obtain the best set of positions all the data must be used and even then there may be errors due to non-convergence. This point will be discussed later.

x

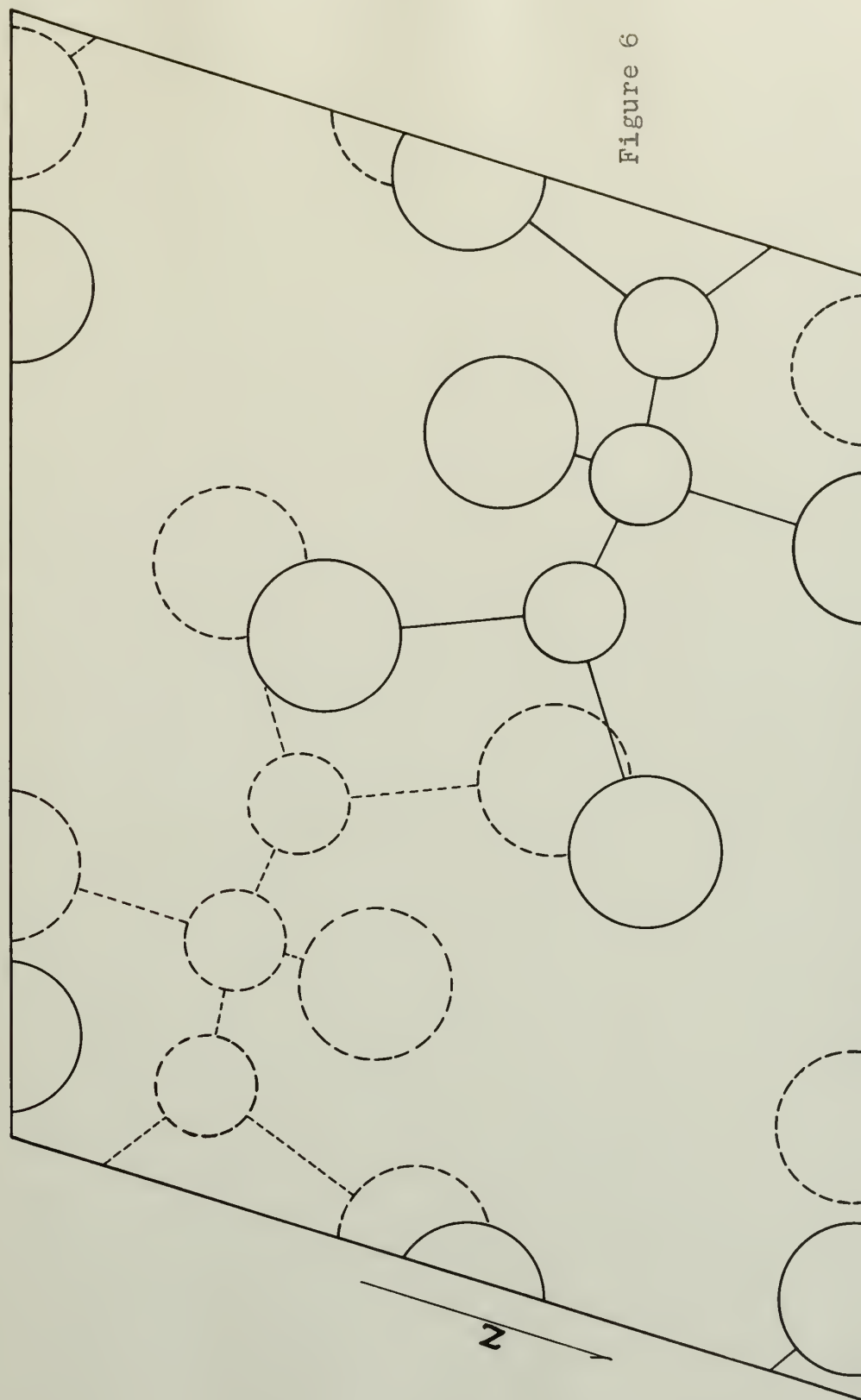


Figure 6

PROJECTION OF UNIT CELL ALONG UNIQUE AXIS

Fourier Sections $\rho(x, 1/4, z)$ and $\rho(1/4, y, z)$.

It is particularly fortunate that half of the atoms of the molecule lie in the symmetry plane $y = 1/4$ and even moreso that the other half lie almost exactly in the plane $x = 1/4$. Thus by taking sections through the unit cell at $y = 1/4$ and at $x = 1/4$ good parameter values should be obtained. This is particularly true since all reflections are used in the syntheses.

The Fourier section $\rho(x, 1/4, z)$ may be evaluated as:

$$\begin{aligned}
 K\rho(x, 1/4, z) = & 4 \sum_{h=1}^{\infty} \sum_{\ell=1}^{\infty} A^1 \cos 2\pi hx \cos 2\pi \ell z \\
 & - 4 \sum_{h=1}^{\infty} \sum_{\ell=1}^{\infty} A^{11} \sin 2\pi hx \sin 2\pi \ell z \\
 & + 4 \sum_{\ell=1}^{\infty} A^{111} \cos 2\pi \ell z + 4 \sum_{h=1}^{\infty} A^{1111} \cos 2\pi hx \\
 & - 4 \sum_{h=1}^{\infty} \sum_{\ell=1}^{\infty} B^1 \cos 2\pi hx \sin 2\pi \ell z \\
 & - 4 \sum_{h=1}^{\infty} \sum_{\ell=1}^{\infty} B^{11} \sin 2\pi hx \cos 2\pi \ell z \\
 & - 4 \sum_{h=1}^{\infty} B^{111} \sin 2\pi hx - 4 \sum_{\ell=1}^{\infty} B^{1111} \sin 2\pi \ell z,
 \end{aligned}$$

(constant additive terms are neglected) where:

$$A^1 = 1/2 (F_{h0\ell} + F_{\bar{h}0\ell}) + \sum_{\substack{k=2n \\ n \geq 1}}^{\infty} (F_{hk\ell} + F_{\bar{h}k\ell}) (-1)^{k/2}.$$

Fourier series $\psi(x, y, z)$ and $\psi(x, y, z)$.

It is particularly fortunate that half of the atoms of the molecule lie in the symmetry plane $y = 1/4$ and even more so that the other half lie almost exactly in the plane $x = 1/4$. Thus by taking sections through the unit cell at $y = 1/4$ and at $x = 1/4$ good parameter values should be obtained. This is particularly true since all reflections are used in the synthesis.

The Fourier section $\psi(x, 1/4, z)$ may be evaluated as

$$\begin{aligned} \psi(x, 1/4, z) &= \sum_{h=1}^{\infty} \sum_{k=1}^{\infty} A_{hk} \cos 2\pi h x \cos 2\pi k z \\ &= \sum_{h=1}^{\infty} \sum_{k=1}^{\infty} A_{hk} \sin 2\pi h x \sin 2\pi k z \\ &= \sum_{h=1}^{\infty} \sum_{k=1}^{\infty} A_{hk} \cos 2\pi h x \sin 2\pi k z \\ &= \sum_{h=1}^{\infty} \sum_{k=1}^{\infty} A_{hk} \sin 2\pi h x \cos 2\pi k z \\ &= \sum_{h=1}^{\infty} \sum_{k=1}^{\infty} A_{hk} \sin 2\pi h x \sin 2\pi k z \end{aligned}$$

(constant additive terms are neglected) where

$$A_{hk} = \sum_{n=1}^{\infty} (F_{hkn} - F_{hkn}^*) / (F_{hkn} + F_{hkn}^*)$$

$$A^{11} = 1/2 (F_{h0l} - F_{h0l}^-) + \sum_{\substack{k=2n \\ n \geq 1}}^{\infty} (F_{hkl} - F_{hkl}^-) (-1)^{k/2},$$

$$A^{111} = 1/2 F_{00l} + \sum_{\substack{k=2n \\ n \geq 1}}^{\infty} F_{0kl} (-1)^{k/2},$$

$$A^{1111} = 1/2 F_{h00} + \sum_{\substack{k=2n \\ n \geq 1}}^{\infty} F_{hko} (-1)^{k/2},$$

$$B^1 = \sum_{\substack{k=2n+1 \\ n \geq 0}}^{\infty} (F_{hkl} + F_{hkl}^-) \left(\sin \frac{\pi k}{2} \right),$$

$$B^{11} = \sum_{\substack{k=2n+1 \\ n \geq 0}}^{\infty} (F_{hkl} - F_{hkl}^-) \left(\sin \frac{\pi k}{2} \right),$$

$$B^{111} = \sum_{\substack{k=2n+1 \\ n \geq 0}}^{\infty} F_{hko} \left(\sin \frac{\pi k}{2} \right),$$

$$B^{1111} = \sum_{\substack{k=2n+1 \\ n \geq 0}}^{\infty} F_{0kl} \left(\sin \frac{\pi k}{2} \right).$$

The section in the plane $x = 1/4$ may be evaluated as (neglecting constant additive terms):

$$K\rho(1/4, y, z) = 4 \sum_{\substack{k=2n \\ n \geq 0}}^{\infty} \sum_{l=1}^{\infty} \left[\sum_{\substack{h=2n \\ n \geq 1}}^{\infty} (F_{hkl} + F_{hkl}^-) \cos \frac{\pi h}{2} \right.$$

$$\left. + F_{0kl} \right] \cos 2\pi ky \cos 2\pi lz$$

$$+ 4 \sum_{\substack{k=2n \\ n \geq 0}}^{\infty} \left[\sum_{\substack{h=2n \\ n \geq 0}}^{\infty} F_{hko} \cos \frac{\pi h}{2} + 1/2 F_{0ko} \right] \cos 2\pi ky$$

$$I_1 = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{2} \right)^n = e^{1/2}$$

$$I_2 = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{2} \right)^n = e^{1/2}$$

$$I_3 = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{2} \right)^n = e^{1/2}$$

$$I_4 = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{2} \right)^n = e^{1/2}$$

$$I_5 = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{2} \right)^n = e^{1/2}$$

$$I_6 = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{2} \right)^n = e^{1/2}$$

$$I_7 = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{2} \right)^n = e^{1/2}$$

The motion in the plane $x = 1/2$ may be evaluated as (neglecting constant additive terms):

$$H(x, y, z) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{2} \right)^n = e^{1/2}$$

$$H(x, y, z) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{2} \right)^n = e^{1/2}$$

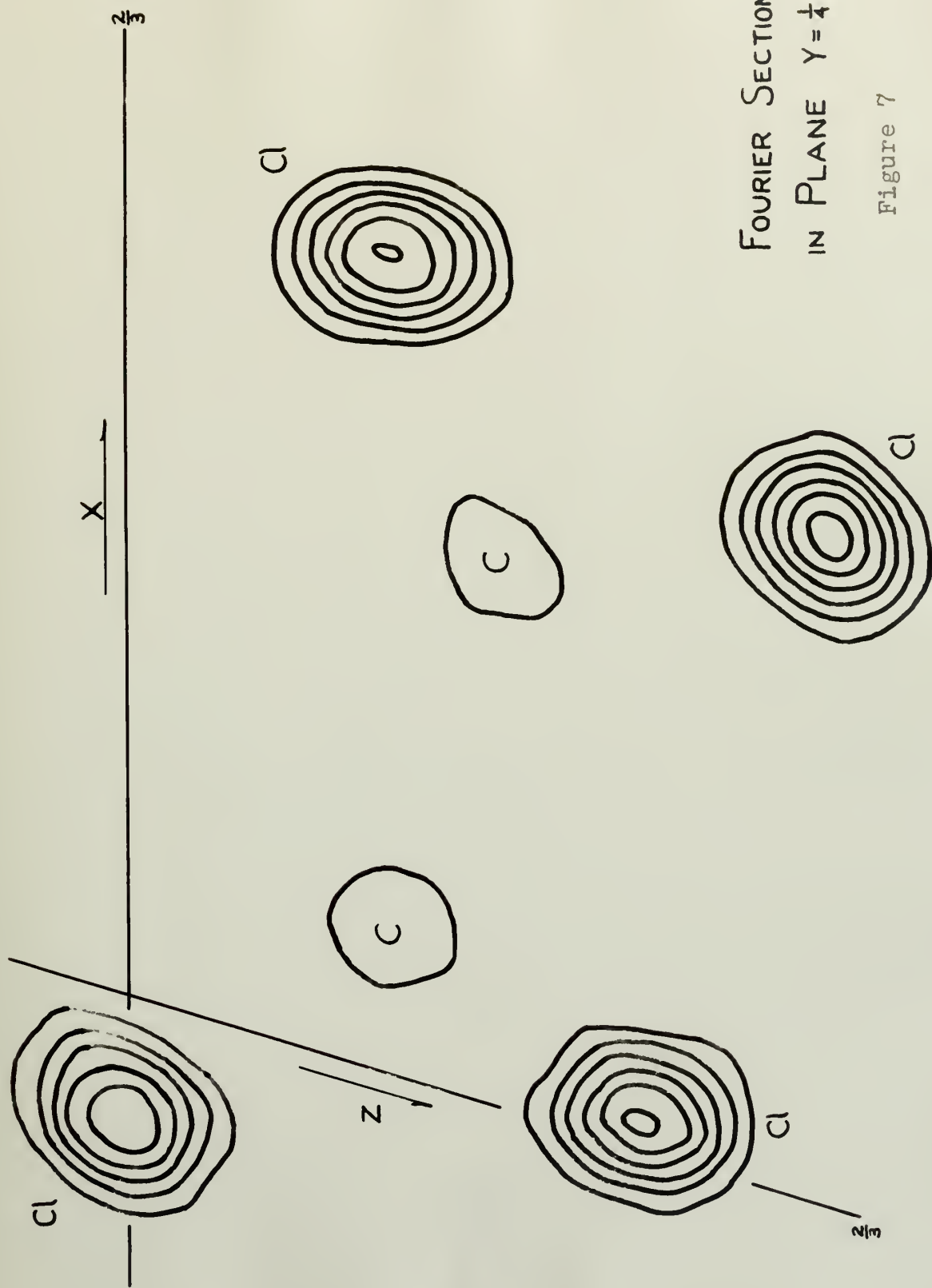
$$H(x, y, z) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{2} \right)^n = e^{1/2}$$

$$\begin{aligned}
& + 4 \sum_{\ell=1}^{\infty} \left[\sum_{\substack{h=2n \\ n \geq 1}}^{\infty} \left(\frac{F_{h0\ell} + F_{\bar{h}0\ell}}{2} \right) \cos \frac{\pi h}{2} + 1/2 F_{00\ell} \right] \cos 2\pi \ell z \\
& - 4 \sum_{\substack{k=2n+1 \\ n \geq 0}}^{\infty} \sum_{\ell=1}^{\infty} \left[F_{0k\ell} + \sum_{\substack{h=2n \\ n \geq 1}}^{\infty} (F_{hk\ell} + F_{\bar{h}k\ell}) \cos \frac{\pi h}{2} \right] \sin 2\pi ky \sin 2\pi \ell z \\
& - 4 \sum_{\substack{k=2n \\ n \geq 0}}^{\infty} \sum_{\ell=1}^{\infty} \left[\sum_{\substack{h=2n+1 \\ n \geq 0}}^{\infty} (F_{hk\ell} - F_{\bar{h}k\ell}) \sin \frac{\pi h}{2} \right. \\
& \left. + \sum_{\substack{h=2n+1 \\ n \geq 0}}^{\infty} \left(\frac{F_{h0\ell} - F_{\bar{h}0\ell}}{2} \right) \sin \frac{\pi h}{2} \right] \cos 2\pi ky \sin 2\pi \ell z \\
& - 4 \sum_{\substack{k=2n+1 \\ n \geq 0}}^{\infty} \sum_{\ell=1}^{\infty} \left[\sum_{\substack{h=2n+1 \\ n \geq 0}}^{\infty} (F_{hk\ell} - F_{\bar{h}k\ell}) \sin \frac{\pi h}{2} \right. \\
& \left. + \sum_{\substack{h=2n+1 \\ n \geq 0}}^{\infty} F_{hk0} \left(\sin \frac{\pi h}{2} \right) \right] \sin 2\pi ky \cos 2\pi \ell z.
\end{aligned}$$

The two Fourier functions were evaluated and appropriate parameters obtained. Phases were recalculated and the final sections are shown in Figures 7 and 8. Contours commence at 25 and are drawn at intervals of 25 units of arbitrary relative electron density. It is readily seen that the carbon positions as given by the weak carbon peaks will not be very accurate. The contours for all atoms were redrawn on large coordinate paper and final atomic coordinates obtained in this study are:

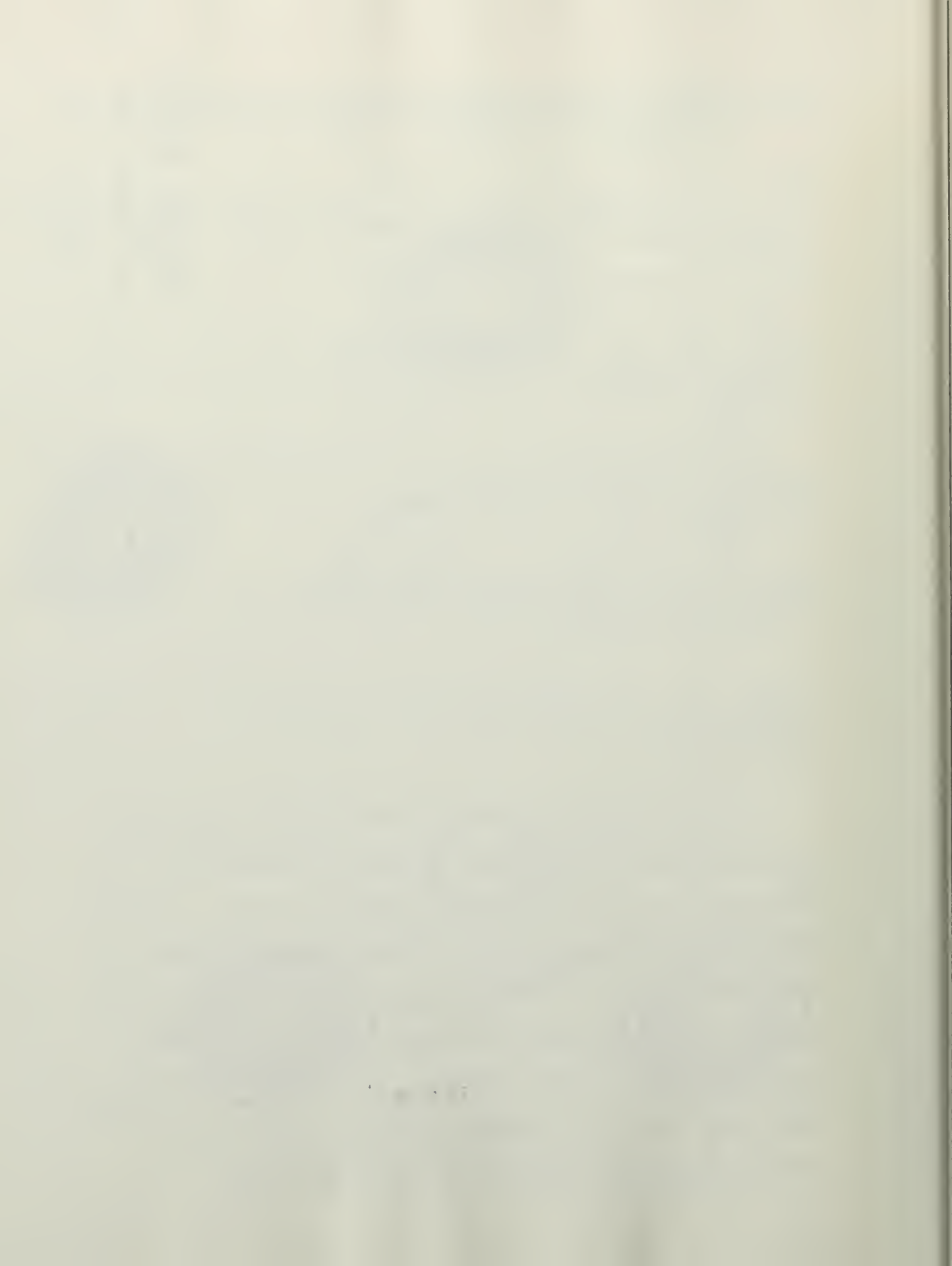
$$\begin{aligned} & \sum_{n=0}^{\infty} \left[\frac{1}{2} \left(\frac{1}{2} \right)^n \cos \left(\frac{n\pi}{2} \right) \right] \\ & \sum_{n=0}^{\infty} \left[\frac{1}{2} \left(\frac{1}{2} \right)^n \sin \left(\frac{n\pi}{2} \right) \right] \\ & \sum_{n=0}^{\infty} \left[\frac{1}{2} \left(\frac{1}{2} \right)^n \cos \left(\frac{n\pi}{2} \right) \right] \\ & \sum_{n=0}^{\infty} \left[\frac{1}{2} \left(\frac{1}{2} \right)^n \sin \left(\frac{n\pi}{2} \right) \right] \\ & \sum_{n=0}^{\infty} \left[\frac{1}{2} \left(\frac{1}{2} \right)^n \cos \left(\frac{n\pi}{2} \right) \right] \\ & \sum_{n=0}^{\infty} \left[\frac{1}{2} \left(\frac{1}{2} \right)^n \sin \left(\frac{n\pi}{2} \right) \right] \end{aligned}$$

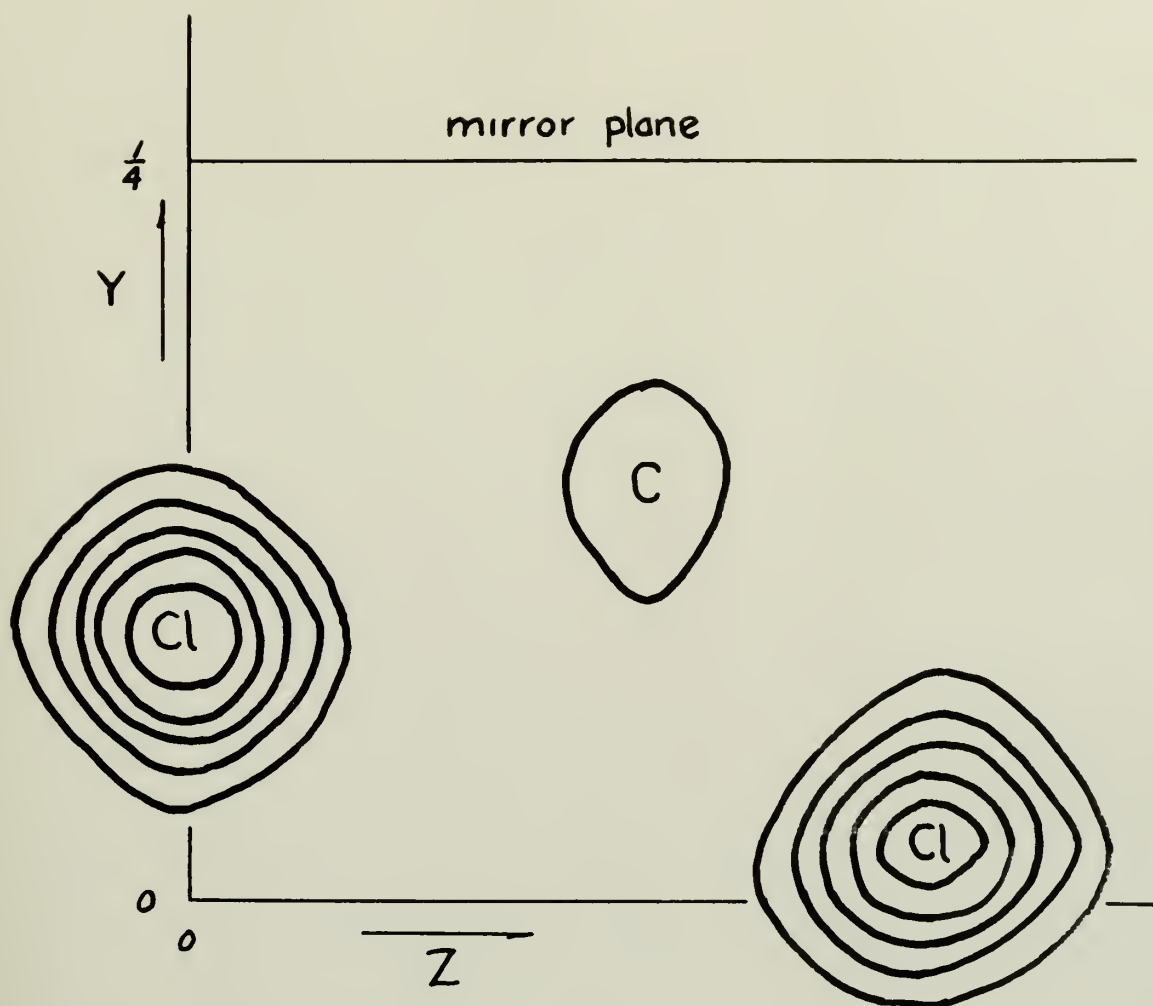
The two Fourier functions were evaluated and approx-
imate parameters obtained. These were recalculated and
the final sections are shown in Figures 7 and 8. Comparing
columns of 10 and are given at intervals of 10 units of
arbitrary relative electron density. It is readily seen
that the carbon positions as given by the wave method
points will not be very accurate. The constants for all
atoms were taken as large constants paper and from
atomic coordinates obtained in this study are



FOURIER SECTION
IN PLANE $Y = \frac{1}{4}$

Figure 7





FOURIER SECTION IN PLANE $x = \frac{1}{4}$

Figure 8



	x	y	z
C ₁	+0.100	1/4	+0.246
C ₂	+0.242	+0.146	+0.264
C ₃	+0.378	1/4	+0.334
C ₁₁	+0.243	+0.091	-0.005
C ₁₄	+0.237	+0.019	+0.425
C ₁₅	+0.462	1/4	+0.638
C ₁₆	+0.022	1/4	+0.465
C ₁₇	-0.084	1/4	-0.006
C ₁₈	+0.564	1/4	+0.242

z	y	x	
590.04	1\1	591.04	10
580.04	591.04	580.04	20
570.04	1\1	570.04	30
560.04	190.04	560.04	40
550.04	510.04	550.04	50
540.04	1\1	540.04	60
530.04	1\1	530.04	70
520.04	1\1	520.04	80
510.04	1\1	510.04	90

COMPARISON OF CALCULATED AND OBSERVED AMPLITUDES

In order to compare calculated and observed amplitudes as a check on the validity of parameters obtained, the effects of thermal motion of the atoms must be considered. While not completely satisfactory an isotropic temperature factor of the form $e^{-B \left(\frac{\sin \theta}{\lambda} \right)^2}$ (where B must be determined) may be used to multiply the amplitudes calculated on the assumption the atoms are at rest in order that a comparison may be made. This is the usual practice in X-ray work. In addition to temperature factor determination it must be remembered that observed amplitudes are on a relative basis. Thus a factor must be determined which will correct them to an absolute scale.

Mathematically then:

$$K |F_{Obs.}| = |F_{calc}| e^{-B \left(\frac{\sin \theta}{\lambda} \right)^2}.$$

This may be rewritten in logarithmic form as

$$\ln \frac{|F_{calc.}|}{|F_{obs.}|} = \ln K + B \left(\frac{\sin \theta}{\lambda} \right)^2$$

which is of the form $y=mx+b$, an equation of a straight line where $b=\ln K$ and $m=B$. The method of least squares was used to determine best values of the slope and intercept of the straight line. It was found that

$$K = 2.87$$

$$B = 2.97 \text{ \AA}^2$$

In order to compare calculated and observed results

as a check on the validity of parameters obtained, the effects of thermal motion of the atoms must be considered. While not completely satisfactory as a check, the calculation of the form factor f_{calc} (where f is the calculated value) may be used to multiply the calculated values for the structure factors and at least in some cases a comparison may be made. This is the usual practice in X-ray work. In addition to temperature factor effects, it must be recognized that observed intensities are on a relative basis. Thus a factor must be determined which will correct them to an absolute scale.

Mathematically then:

$$R = \frac{|F_{obs}|}{|F_{calc}|} = \frac{|F_{calc}|}{|F_{calc}|} = 1$$

This may be rewritten in logarithmic form as

$$\ln \left| \frac{F_{obs}}{F_{calc}} \right| = \ln R = \ln \left| \frac{F_{calc}}{F_{calc}} \right|$$

which is of the form $y = mx + b$, an equation of a straight line where y and x are. The method of least squares was used to determine best values of the slope and intercept of the straight line. It was found that

$$R = 1.17$$

$$R = 1.17 \pm 0.05$$

when the 592 forms were used in the calculation.

Table I lists $\frac{(F_{\text{calc.}})}{2} e^{-3\left(\frac{\sin \theta}{\lambda}\right)^2}$ and $2.87 F_{\text{obs.}}$

for each reflection;

TABLE I

$\frac{F_{hkl}}{2}$			$\frac{F_{hkl}}{2}$		
hkl	Calc.	Obs.	hkl	Calc.	Obs.
020	-29.0	35.0	300	- 9.5	11.5
040	+47.6	53.9	310	+21.6	25.0
060	-34.1	37.6	320	- 4.2	4.0
080	+30.4	31.5	330	+20.6	24.1
0,10,0	- 9.8	4.9	340	- 2.5	0
0,12,0	+16.7	18.3	350	+11.9	12.3
			360	- 0.2	0
100	+ 4.2	4.6	370	- 3.1	0
110	-25.5	28.4	380	- 1.9	0
120	+ 2.8	3.4	390	+ 3.3	0
130	-36.6	32.7	3,10,0	- 0.7	0
140	+ 0.5	0	3,11,0	+ 3.2	2.9
150	- 8.3	11.5	3,12,0	- 0.9	0
160	+0.5	0	3,13,0	+ 7.1	6.0
170	- 1.1	0			
180	+ 0.4	0	400	+38.1	45.6
190	- 0.3	0	410	+ 3.1	3.7
1,10,0	+ 0.5	0	420	+16.3	18.1
1,11,0	- 6.2	6.6	430	+ 4.0	4.6
1,12,0	+ 0.2	0	440	+ 2.6	5.2
1,13,0	- 6.6	9.5	450	+ 2.5	0
			460	- 2.5	0
200	-18.6	18.7	470	- 0.3	0
210	+ 2.2	2.3	480	+ 6.0	7.2
220	-68.2	57.5	490	+ 1.8	0
230	- 6.8	8.6	4,10,0	+ 4.3	4.6
240	+27.9	32.1	4,11,0	+ 1.3	0
250	+ 1.4	0	4,12,0	+ 4.5	4.3
260	-20.2	24.1			
270	- 8.8	0	500	+ 8.2	9.5
280	+ 9.8	8.6	510	-10.7	10.6
290	+ 0.5	0	520	+ 6.2	4.9
2,10,0	-18.2	20.7	530	-15.8	16.3
2,11,0	- 1.9	0	540	+ 1.4	0
2,12,0	+ 3.0	0	550	- 5.7	5.5
2,13,0	- 0.2	0	560	+ 1.4	0

where the 75% value was used in the calculation.

$$= \frac{1}{2} \left(\frac{1}{1} + \frac{1}{1} \right) = 1$$

1000 700 600 500 400 300 200 100 0

ACKNOWLEDGMENTS

[illegible]

TABLE I (Continued)

hk ℓ	Calc.	Obs.	hk ℓ	Calc.	Obs.
570	+ 0.4	0	950	- 7.8	8.0
580	+ 1.4	0	001	- 7.9	10.0
590	- 0.7	0	011	-22.9	22.4
5,10,0	+ 1.5	0	021	- 2.1	1.6
5,11,0	- 3.3	0	031	+ 5.4	6.6
600	-26.7	31.0	041	-35.0	35.6
610	- 7.0	6.0	051	- 6.8	5.2
620	- 6.3	4.6	061	-18.3	18.1
630	- 1.9	0	071	- 0.6	0
640	- 4.7	6.3	081	-10.5	10.6
650	- 4.2	4.0	091	- 9.8	8.3
660	+ 5.1	4.6	0,10,1	+ 6.4	0
670	+ 1.7	0	0,11,1	+ 0.7	0
680	- 6.1	7.2	0,12,1	+ 1.8	0
690	- 2.4	0	0,13,1	- 3.0	0
6,10,0	- 1.5	0	101	-10.9	6.6
6,11,0	+ 0.8	0	111	- 1.0	2.3
700	- 4.9	2.9	121	-19.5	21.2
710	- 0.3	0	131	-23.2	25.0
720	- 7.4	6.0	141	+ 2.0	2.3
730	+15.5	13.2	151	+ 9.9	7.8
740	+ 0.8	0	161	-14.3	14.4
750	- 2.0	0	171	+11.9	11.2
760	- 2.8	4.6	181	- 3.6	0
770	+ 4.2	0	191	+17.8	16.1
780	- 0.1	0	1,10,1	- 2.5	2.9
790	- 2.9	0	1,11,1	+ 2.4	0
800	+ 9.4	7.2	1,12,1	+ 2.1	0
810	+ 0.4	0	1,13,1	+ 1.4	0
820	+ 9.4	9.5	I01	+28.0	32.8
830	+ 5.0	5.5	I11	- 2.5	0
840	- 3.0	4.0	I21	+ 2.6	2.9
850	+ 0.4	0	I31	+26.6	26.2
860	+ 1.4	0	I41	+ 3.8	6.9
870	+ 1.0	0	I51	-11.8	9.2
880	+0	0	I61	+ 3.7	4.0
900	+ 9.9	10.9	I71	-12.3	11.5
910	-10.8	13.8	I81	+ 5.5	4.6
920	- 0.7	3.4	I91	-19.8	16.6
930	+ 1.7	4.6	I,10,1	- 1.7	0
940	+ 4.8	5.7	I,11,1	- 2.5	0
			I,12,1	+ 0.9	0

Table 1 (Continued)

Age	Sex	Year	Age	Sex	Year
0.0	M	1900	0.0	F	1900
0.0	M	1901	0.0	F	1901
0.0	M	1902	0.0	F	1902
0.0	M	1903	0.0	F	1903
0.0	M	1904	0.0	F	1904
0.0	M	1905	0.0	F	1905
0.0	M	1906	0.0	F	1906
0.0	M	1907	0.0	F	1907
0.0	M	1908	0.0	F	1908
0.0	M	1909	0.0	F	1909
0.0	M	1910	0.0	F	1910
0.0	M	1911	0.0	F	1911
0.0	M	1912	0.0	F	1912
0.0	M	1913	0.0	F	1913
0.0	M	1914	0.0	F	1914
0.0	M	1915	0.0	F	1915
0.0	M	1916	0.0	F	1916
0.0	M	1917	0.0	F	1917
0.0	M	1918	0.0	F	1918
0.0	M	1919	0.0	F	1919
0.0	M	1920	0.0	F	1920
0.0	M	1921	0.0	F	1921
0.0	M	1922	0.0	F	1922
0.0	M	1923	0.0	F	1923
0.0	M	1924	0.0	F	1924
0.0	M	1925	0.0	F	1925
0.0	M	1926	0.0	F	1926
0.0	M	1927	0.0	F	1927
0.0	M	1928	0.0	F	1928
0.0	M	1929	0.0	F	1929
0.0	M	1930	0.0	F	1930
0.0	M	1931	0.0	F	1931
0.0	M	1932	0.0	F	1932
0.0	M	1933	0.0	F	1933
0.0	M	1934	0.0	F	1934
0.0	M	1935	0.0	F	1935
0.0	M	1936	0.0	F	1936
0.0	M	1937	0.0	F	1937
0.0	M	1938	0.0	F	1938
0.0	M	1939	0.0	F	1939
0.0	M	1940	0.0	F	1940
0.0	M	1941	0.0	F	1941
0.0	M	1942	0.0	F	1942
0.0	M	1943	0.0	F	1943
0.0	M	1944	0.0	F	1944
0.0	M	1945	0.0	F	1945
0.0	M	1946	0.0	F	1946
0.0	M	1947	0.0	F	1947
0.0	M	1948	0.0	F	1948
0.0	M	1949	0.0	F	1949
0.0	M	1950	0.0	F	1950
0.0	M	1951	0.0	F	1951
0.0	M	1952	0.0	F	1952
0.0	M	1953	0.0	F	1953
0.0	M	1954	0.0	F	1954
0.0	M	1955	0.0	F	1955
0.0	M	1956	0.0	F	1956
0.0	M	1957	0.0	F	1957
0.0	M	1958	0.0	F	1958
0.0	M	1959	0.0	F	1959
0.0	M	1960	0.0	F	1960
0.0	M	1961	0.0	F	1961
0.0	M	1962	0.0	F	1962
0.0	M	1963	0.0	F	1963
0.0	M	1964	0.0	F	1964
0.0	M	1965	0.0	F	1965
0.0	M	1966	0.0	F	1966
0.0	M	1967	0.0	F	1967
0.0	M	1968	0.0	F	1968
0.0	M	1969	0.0	F	1969
0.0	M	1970	0.0	F	1970
0.0	M	1971	0.0	F	1971
0.0	M	1972	0.0	F	1972
0.0	M	1973	0.0	F	1973
0.0	M	1974	0.0	F	1974
0.0	M	1975	0.0	F	1975
0.0	M	1976	0.0	F	1976
0.0	M	1977	0.0	F	1977
0.0	M	1978	0.0	F	1978
0.0	M	1979	0.0	F	1979
0.0	M	1980	0.0	F	1980
0.0	M	1981	0.0	F	1981
0.0	M	1982	0.0	F	1982
0.0	M	1983	0.0	F	1983
0.0	M	1984	0.0	F	1984
0.0	M	1985	0.0	F	1985
0.0	M	1986	0.0	F	1986
0.0	M	1987	0.0	F	1987
0.0	M	1988	0.0	F	1988
0.0	M	1989	0.0	F	1989
0.0	M	1990	0.0	F	1990
0.0	M	1991	0.0	F	1991
0.0	M	1992	0.0	F	1992
0.0	M	1993	0.0	F	1993
0.0	M	1994	0.0	F	1994
0.0	M	1995	0.0	F	1995
0.0	M	1996	0.0	F	1996
0.0	M	1997	0.0	F	1997
0.0	M	1998	0.0	F	1998
0.0	M	1999	0.0	F	1999
0.0	M	2000	0.0	F	2000

TABLE I (Continued)

hk λ	Calc.	Obs.	hk λ	Calc.	Obs.
<u>1</u> ,13,1	- 2.1	0	<u>3</u> 01	-27.6	33.0
201	-29.2	30.8	<u>3</u> 11	-33.2	31.6
211	+ 8.7	8.9	<u>3</u> 21	+ 9.9	8.9
221	+29.5	34.7	<u>3</u> 31	+10.4	9.2
231	- 0.2	0	<u>3</u> 41	-10.7	10.8
241	+ 4.5	5.5	<u>3</u> 51	-13.8	12.9
251	+ 3.6	0	<u>3</u> 61	+ 6.4	4.6
261	+33.8	30.1	<u>3</u> 71	+29.2	24.4
271	+ 3.9	0	<u>3</u> 81	- 9.4	5.7
281	- 5.0	0	<u>3</u> 91	+ 4.6	0
291	+ 8.5	6.6	<u>3</u> ,10,1	+ 5.4	0
2,10,1	+ 4.0	0	<u>3</u> ,11,1	+11.5	9.8
2,11,1	+ 1.5	0	<u>3</u> ,12,1	- 2.7	0
2,12,1	- 8.7	4.6	<u>3</u> ,13,1	- 4.4	0
2,13,1	+ 1.9	0			
<u>2</u> 01	+ 2.3	0	401	-20.2	28.1
<u>2</u> 11	- 4.4	4.0	411	+ 7.9	10.6
<u>2</u> 21	+ 9.5	9.2	421	+20.2	25.5
<u>2</u> 31	+15.7	16.4	431	-11.0	11.8
<u>2</u> 41	+28.2	30.4	441	-35.2	40.2
<u>2</u> 51	- 8.3	7.5	451	+ 6.3	8.9
<u>2</u> 61	+21.8	20.6	461	+ 3.1	4.0
<u>2</u> 71	+ 8.0	7.8	471	-12.3	11.2
<u>2</u> 81	+7.9	8.3	481	-17.8	14.4
<u>2</u> 91	- 0.3	3.7	491	- 2.1	0
2,10,1	- 4.4	0	4,10,1	+12.1	8.9
2,11,1	+ 3.9	0	4,11,1	- 6.0	5.2
2,12,1	- 3.0	0	4,12,1	- 3.9	0
2,13,1	- 1.2	0			
301	+16.7	15.8	<u>4</u> 01	+ 1.5	0
311	+20.4	25.6	<u>4</u> 11	- 5.4	5.7
321	+ 5.5	4.9	<u>4</u> 21	-10.8	11.5
331	+ 0.5	0	<u>4</u> 31	- 3.3	4.0
341	+ 9.7	9.8	<u>4</u> 41	-18.5	16.6
351	+ 6.7	6.9	<u>4</u> 51	+ 0.6	0
361	+ 6.5	8.0	<u>4</u> 61	-20.0	18.7
371	-19.7	17.8	<u>4</u> 71	+ 0.2	0
381	+ 6.6	5.7	<u>4</u> 81	- 5.0	4.0
391	- 6.1	6.6	491	- 1.9	0
3,10,1	- 2.0	0	4,10,1	+ 2.3	0
3,11,1	- 7.2	8.9	4,11,1	+ 0.1	0
3,12,1	+ 0.5	0	4,12,1	+ 3.5	0

TABLE 1 (continued)

Code	Code	Code	Code	Code	Code
C.11	A.11	100	0	1.1	1.01,1
C.12	C.12	110	A.12	2.1	1.02,1
P.1	P.1	120	P.1	3.1	1.03,1
C.1	H.01	130	T.1	C.1	1.04,1
C.01	T.01	140	0	C.1	1.05,1
P.1	H.11	150	C.1	C.1	1.06,1
C.1	A.1	160	0	C.1	1.07,1
C.1	C.1	170	A.1	C.1	1.08,1
T.1	A.1	180	0	C.1	1.09,1
0	A.1	190	0	C.1	1.10,1
0	A.1	1.01,1	0	C.1	1.11,1
C.1	C.1	1.11,1	0	C.1	1.12,1
0	T.1	1.11,1	0	C.1	1.13,1
0	H.1	1.11,1	0	C.1	1.14,1
1.1	T.1	1.11,1	0	C.1	1.15,1
0.01	P.1	1.11,1	0	C.1	1.16,1
P.1	C.1	1.11,1	0	C.1	1.17,1
C.1	C.1	1.11,1	0	C.1	1.18,1
T.1	C.1	1.11,1	0	C.1	1.19,1
P.1	C.1	1.11,1	0	C.1	1.20,1
C.1	C.1	1.11,1	0	C.1	1.21,1
C.1	C.1	1.11,1	0	C.1	1.22,1
A.1	C.1	1.11,1	0	C.1	1.23,1
0	C.1	1.11,1	0	C.1	1.24,1
C.1	C.1	1.11,1	0	C.1	1.25,1
0	C.1	1.11,1	0	C.1	1.26,1
0	C.1	1.11,1	0	C.1	1.27,1
0	C.1	1.11,1	0	C.1	1.28,1
0	C.1	1.11,1	0	C.1	1.29,1
0	C.1	1.11,1	0	C.1	1.30,1
0	C.1	1.11,1	0	C.1	1.31,1
0	C.1	1.11,1	0	C.1	1.32,1
0	C.1	1.11,1	0	C.1	1.33,1
0	C.1	1.11,1	0	C.1	1.34,1
0	C.1	1.11,1	0	C.1	1.35,1
0	C.1	1.11,1	0	C.1	1.36,1
0	C.1	1.11,1	0	C.1	1.37,1
0	C.1	1.11,1	0	C.1	1.38,1
0	C.1	1.11,1	0	C.1	1.39,1
0	C.1	1.11,1	0	C.1	1.40,1
0	C.1	1.11,1	0	C.1	1.41,1
0	C.1	1.11,1	0	C.1	1.42,1
0	C.1	1.11,1	0	C.1	1.43,1
0	C.1	1.11,1	0	C.1	1.44,1
0	C.1	1.11,1	0	C.1	1.45,1
0	C.1	1.11,1	0	C.1	1.46,1
0	C.1	1.11,1	0	C.1	1.47,1
0	C.1	1.11,1	0	C.1	1.48,1
0	C.1	1.11,1	0	C.1	1.49,1
0	C.1	1.11,1	0	C.1	1.50,1

TABLE I (Continued)

hk ℓ	Calc.	Obs.	hk ℓ	Calc.	Obs.
501	- 8.3	9.5	<u>661</u>	+14.2	11.8
511	- 1.5	0	<u>671</u>	- 7.2	0
521	- 6.8	4.6	<u>681</u>	+ 4.0	0
531	-11.5	12.3	<u>691</u>	+ 2.1	0
541	- 6.0	6.6	<u>6,10,1</u>	- 2.0	0
551	+ 4.4	5.2	<u>6,11,1</u>	- 1.9	0
561	- 8.2	8.0			
571	+ 6.2	0	701	+ 5.0	0
581	- 3.7	0	711	+ 3.2	0
591	+ 9.1	7.5	721	+ 4.9	0
5,10,1	+ 0.5	0	731	+ 5.6	0
5,11,1	+ 1.0	0	741	+ 4.4	4.3
			751	- 0.8	0
<u>501</u>	-14.4	19.2	761	+ 6.2	6.3
<u>511</u>	-11.8	15.5	771	- 4.8	0
<u>521</u>	+21.1	27.0	781	+ 2.6	0
<u>531</u>	+22.8	23.0	791	- 4.4	0
<u>541</u>	-20.0	20.6			
<u>551</u>	-14.9	14.1	<u>701</u>	-15.0	21.5
<u>561</u>	+14.6	14.6	<u>711</u>	-10.1	11.8
<u>571</u>	- 2.6	0	<u>721</u>	+11.2	11.2
<u>581</u>	-10.0	6.6	<u>731</u>	+ 2.1	0
<u>591</u>	-18.2	14.6	<u>741</u>	- 6.4	8.6
<u>5,10,1</u>	+ 8.0	0	<u>751</u>	- 4.3	5.7
<u>5,11,1</u>	+ 1.4	0	<u>761</u>	+ 9.5	9.8
<u>5,12,1</u>	- 5.3	0	<u>771</u>	+12.6	9.8
			<u>781</u>	- 6.6	7.8
601	-19.8	24.6	<u>791</u>	+ 3.1	2.6
611	+ 5.4	5.2	<u>7,10,1</u>	+ 5.0	0
621	+16.5	22.6			
631	- 3.2	5.5	801	- 0.6	0
641	- 4.0	6.3	811	- 1.2	0
651	+ 4.7	4.6	821	+ 1.6	4.6
661	+19.8	19.2	831	+ 0.5	3.4
671	+ 2.1	0	841	- 8.6	8.6
681	- 6.4	7.2	851	- 1.6	0
691	+ 7.7	7.5	861	- 1.7	2.9
6,10,1	+ 4.5	4.0	871	- 2.8	0
<u>601</u>	+ 0.1	0	<u>801</u>	- 1.8	0
<u>611</u>	+ 7.3	7.7	<u>811</u>	+ 1.0	0
<u>621</u>	+ 6.6	5.5	<u>821</u>	- 2.7	0
<u>631</u>	- 0.7	4.0	<u>831</u>	- 5.2	5.2
<u>641</u>	+12.9	11.2	<u>841</u>	- 8.8	6.9
<u>651</u>	+ 2.0	0	<u>851</u>	+ 3.6	3.4

Year	Value	Index	Year	Value	Index
1911	1.11	100	1921	1.11	100
1912	1.12	101	1922	1.12	101
1913	1.13	102	1923	1.13	102
1914	1.14	103	1924	1.14	103
1915	1.15	104	1925	1.15	104
1916	1.16	105	1926	1.16	105
1917	1.17	106	1927	1.17	106
1918	1.18	107	1928	1.18	107
1919	1.19	108	1929	1.19	108
1920	1.20	109	1930	1.20	109
1921	1.21	110	1931	1.21	110
1922	1.22	111	1932	1.22	111
1923	1.23	112	1933	1.23	112
1924	1.24	113	1934	1.24	113
1925	1.25	114	1935	1.25	114
1926	1.26	115	1936	1.26	115
1927	1.27	116	1937	1.27	116
1928	1.28	117	1938	1.28	117
1929	1.29	118	1939	1.29	118
1930	1.30	119	1940	1.30	119
1931	1.31	120	1941	1.31	120
1932	1.32	121	1942	1.32	121
1933	1.33	122	1943	1.33	122
1934	1.34	123	1944	1.34	123
1935	1.35	124	1945	1.35	124
1936	1.36	125	1946	1.36	125
1937	1.37	126	1947	1.37	126
1938	1.38	127	1948	1.38	127
1939	1.39	128	1949	1.39	128
1940	1.40	129	1950	1.40	129
1941	1.41	130	1951	1.41	130
1942	1.42	131	1952	1.42	131
1943	1.43	132	1953	1.43	132
1944	1.44	133	1954	1.44	133
1945	1.45	134	1955	1.45	134
1946	1.46	135	1956	1.46	135
1947	1.47	136	1957	1.47	136
1948	1.48	137	1958	1.48	137
1949	1.49	138	1959	1.49	138
1950	1.50	139	1960	1.50	139
1951	1.51	140	1961	1.51	140
1952	1.52	141	1962	1.52	141
1953	1.53	142	1963	1.53	142
1954	1.54	143	1964	1.54	143
1955	1.55	144	1965	1.55	144
1956	1.56	145	1966	1.56	145
1957	1.57	146	1967	1.57	146
1958	1.58	147	1968	1.58	147
1959	1.59	148	1969	1.59	148
1960	1.60	149	1970	1.60	149
1961	1.61	150	1971	1.61	150
1962	1.62	151	1972	1.62	151
1963	1.63	152	1973	1.63	152
1964	1.64	153	1974	1.64	153
1965	1.65	154	1975	1.65	154
1966	1.66	155	1976	1.66	155
1967	1.67	156	1977	1.67	156
1968	1.68	157	1978	1.68	157
1969	1.69	158	1979	1.69	158
1970	1.70	159	1980	1.70	159
1971	1.71	160	1981	1.71	160
1972	1.72	161	1982	1.72	161
1973	1.73	162	1983	1.73	162
1974	1.74	163	1984	1.74	163
1975	1.75	164	1985	1.75	164
1976	1.76	165	1986	1.76	165
1977	1.77	166	1987	1.77	166
1978	1.78	167	1988	1.78	167
1979	1.79	168	1989	1.79	168
1980	1.80	169	1990	1.80	169
1981	1.81	170	1991	1.81	170

TABLE I (Continued)

hk ℓ	Calc.	Obs.	hk ℓ	Calc.	Obs.
<u>861</u>	- 7.7	5.2	192	+11.7	8.3
<u>871</u>	- 0.5	0	1,10,2	- 6.2	0
<u>881</u>	- 3.5	3.1	1,11,2	- 7.8	6.3
901	- 4.1	0	1,12,2	+ 7.0	5.5
911	- 2.3	0	1,13,2	- 2.9	3.4
921	- 1.6	0	<u>102</u>	+12.5	16.1
931	- 3.0	0	<u>112</u>	+20.9	21.0
941	- 4.0	0	<u>122</u>	-44.5	44.8
<u>901</u>	+ 0.5	0	<u>132</u>	+10.3	13.8
<u>911</u>	- 1.2	0	<u>142</u>	+12.0	12.1
<u>921</u>	- 0.3	0	<u>152</u>	+21.6	18.1
<u>931</u>	+ 5.1	4.0	<u>162</u>	-25.7	21.0
<u>941</u>	- 3.9	5.4	<u>172</u>	-10.1	7.5
<u>951</u>	- 3.0	0	<u>182</u>	+ 9.0	0
<u>961</u>	- 0.6	0	<u>192</u>	- 0.2	0
<u>10,0,1</u>	+ 2.2	0	1,10,2	-11.5	10.6
<u>10,1,1</u>	+ 1.5	0	1,11,2	+ 1.1	0
<u>10,2,1</u>	+ 1.0	0	1,12,2	+ 6.1	0
002	+32.6	38.4	1,13,2	+ 9.1	7.5
012	+ 0.1	0	202	-14.6	13.5
022	+18.1	21.2	212	+ 5.4	4.9
032	+ 9.4	10.1	222	-19.5	21.8
042	+ 4.0	5.2	232	-14.3	15.5
052	+ 4.7	2.9	242	+ 5.5	4.0
062	-11.6	11.8	252	- 1.0	0
072	+ 8.0	5.2	262	+ 4.9	4.9
082	+ 2.3	0	272	-10.2	3.4
092	+ 4.2	3.4	282	+ 3.0	0
0,10,2	+ 7.5	7.2	292	- 1.1	0
0,11,2	+ 5.4	5.7	2,10,2	- 9.4	7.8
0,12,2	+ 5.4	4.3	2,11,2	- 6.9	4.6
0,13,2	+ 2.8	4.0	2,12,2	- 2.6	0
102	+46.0	46.5	<u>202</u>	-28.2	33.0
112	+ 8.1	9.8	<u>212</u>	-22.0	22.4
122	- 8.2	9.2	<u>222</u>	-24.9	28.4
132	-32.2	31.8	<u>232</u>	+12.6	11.8
142	+32.7	31.0	<u>242</u>	- 1.3	0
152	+ 0.4	0	<u>252</u>	-18.4	12.9
162	- 9.5	7.2	<u>262</u>	+ 6.2	5.2
172	- 4.1	0	<u>272</u>	+ 3.9	2.3
182	+16.5	15.2	<u>282</u>	- 0.2	0
			<u>292</u>	-12.9	9.5
			2,10,2	- 9.8	8.6

TABLE 2 (Continued)

Year	Age	Sex	Year	Age	Sex
1950	7.11	Male	1950	7.7	Male
1951	7.11	Male	1951	7.7	Male
1952	7.11	Male	1952	7.7	Male
1953	7.11	Male	1953	7.7	Male
1954	7.11	Male	1954	7.7	Male
1955	7.11	Male	1955	7.7	Male
1956	7.11	Male	1956	7.7	Male
1957	7.11	Male	1957	7.7	Male
1958	7.11	Male	1958	7.7	Male
1959	7.11	Male	1959	7.7	Male
1960	7.11	Male	1960	7.7	Male
1961	7.11	Male	1961	7.7	Male
1962	7.11	Male	1962	7.7	Male
1963	7.11	Male	1963	7.7	Male
1964	7.11	Male	1964	7.7	Male
1965	7.11	Male	1965	7.7	Male
1966	7.11	Male	1966	7.7	Male
1967	7.11	Male	1967	7.7	Male
1968	7.11	Male	1968	7.7	Male
1969	7.11	Male	1969	7.7	Male
1970	7.11	Male	1970	7.7	Male
1971	7.11	Male	1971	7.7	Male
1972	7.11	Male	1972	7.7	Male
1973	7.11	Male	1973	7.7	Male
1974	7.11	Male	1974	7.7	Male
1975	7.11	Male	1975	7.7	Male
1976	7.11	Male	1976	7.7	Male
1977	7.11	Male	1977	7.7	Male
1978	7.11	Male	1978	7.7	Male
1979	7.11	Male	1979	7.7	Male
1980	7.11	Male	1980	7.7	Male
1981	7.11	Male	1981	7.7	Male
1982	7.11	Male	1982	7.7	Male
1983	7.11	Male	1983	7.7	Male
1984	7.11	Male	1984	7.7	Male
1985	7.11	Male	1985	7.7	Male
1986	7.11	Male	1986	7.7	Male
1987	7.11	Male	1987	7.7	Male
1988	7.11	Male	1988	7.7	Male
1989	7.11	Male	1989	7.7	Male
1990	7.11	Male	1990	7.7	Male
1991	7.11	Male	1991	7.7	Male
1992	7.11	Male	1992	7.7	Male
1993	7.11	Male	1993	7.7	Male
1994	7.11	Male	1994	7.7	Male
1995	7.11	Male	1995	7.7	Male
1996	7.11	Male	1996	7.7	Male
1997	7.11	Male	1997	7.7	Male
1998	7.11	Male	1998	7.7	Male
1999	7.11	Male	1999	7.7	Male
2000	7.11	Male	2000	7.7	Male

TABLE 1 (Continued)

hk ℓ	Calc.	Obs.	hk ℓ	Calc.	Obs.
$\bar{2},11,2$	+ 1.4	0	$\bar{4}02$	+22.2	26.1
$\bar{2},12,2$	- 4.0	3.7	$\bar{4}12$	-13.4	14.6
$\bar{2},13,2$	- 6.0	5.2	$\bar{4}22$	+21.8	19.5
302	- 9.1	7.5	$\bar{4}32$	+14.2	14.1
312	+21.1	20.1	$\bar{4}42$	+ 0.9	3.1
322	-19.9	22.4	$\bar{4}52$	- 7.8	9.8
332	- 1.3	0	$\bar{4}62$	- 3.2	4.9
342	- 3.2	0	$\bar{4}72$	+13.0	10.0
352	+19.4	16.1	$\bar{4}82$	0	0
362	- 9.4	7.5	$\bar{4}92$	- 1.4	0
372	-14.0	7.8	$\bar{4},10,2$	+ 8.8	8.3
382	- 0.3	0	$\bar{4},11,2$	+ 7.0	5.7
392	- 2.0	0	$\bar{4},12,2$	+ 3.2	3.7
$3,10,2$	- 5.3	4.0	502	+ 6.0	0
$3,11,2$	- 3.0	0	512	- 3.9	4.9
$3,12,2$	+ 0.6	0	522	+15.6	16.9
$\bar{3}02$	+27.0	36.0	532	- 7.7	8.6
$\bar{3}12$	+ 2.8	4.6	542	+ 1.3	0
$\bar{3}22$	- 3.5	5.2	552	- 4.9	0
$\bar{3}32$	-28.8	29.3	562	+ 7.1	6.9
$\bar{3}42$	+20.8	21.0	572	+ 4.1	0
$\bar{3}52$	- 4.3	6.0	582	- 0.4	0
$\bar{3}62$	- 2.4	4.0	592	+ 4.1	0
$\bar{3}72$	- 3.6	0	$5,10,2$	+ 5.0	5.2
$\bar{3}82$	+10.7	10.9	$\bar{5}02$	- 3.8	2.3
$\bar{3}92$	+ 7.8	5.7	$\bar{5}12$	+17.6	18.4
$\bar{3},10,2$	- 4.2	0	$\bar{5}22$	- 7.6	8.6
$\bar{3},11,2$	- 7.6	7.2	$\bar{5}32$	+ 3.9	3.7
$\bar{3},12,2$	+ 3.7	0	$\bar{5}42$	- 3.9	0
$3,13,2$	- 4.8	0	$\bar{5}52$	+18.3	20.1
402	+20.2	20.4	$\bar{5}62$	- 6.8	8.9
412	+10.3	8.3	$\bar{5}72$	- 8.2	6.9
422	+ 0.3	0	$\bar{5}82$	- 1.4	0
432	- 1.5	0	$\bar{5}92$	+ 2.8	0
442	+ 5.0	5.7	$\bar{5},10,2$	- 0.8	0
452	+12.5	8.6	$\bar{5},11,2$	+ 0.4	0
462	-13.1	10.4	$\bar{5},12,2$	+ 0.8	0
472	- 1.3	0	602	+ 1.3	6.0
482	+ 3.7	0	612	- 2.3	0
492	+ 7.1	0	622	-11.6	12.6
$4,10,2$	+ 1.7	0	632	- 4.0	2.9
$4,11,2$	+ 1.0	0	642	+ 9.2	5.7

TABLE 1. (continued)

Year	Value	Unit	Year	Value	Unit
1971	2.35	kg	1971	0.1	kg
1972	2.15	kg	1972	0.1	kg
1973	2.15	kg	1973	0.1	kg
1974	2.15	kg	1974	0.1	kg
1975	2.15	kg	1975	0.1	kg
1976	2.15	kg	1976	0.1	kg
1977	2.15	kg	1977	0.1	kg
1978	2.15	kg	1978	0.1	kg
1979	2.15	kg	1979	0.1	kg
1980	2.15	kg	1980	0.1	kg
1981	2.15	kg	1981	0.1	kg
1982	2.15	kg	1982	0.1	kg
1983	2.15	kg	1983	0.1	kg
1984	2.15	kg	1984	0.1	kg
1985	2.15	kg	1985	0.1	kg
1986	2.15	kg	1986	0.1	kg
1987	2.15	kg	1987	0.1	kg
1988	2.15	kg	1988	0.1	kg
1989	2.15	kg	1989	0.1	kg
1990	2.15	kg	1990	0.1	kg
1991	2.15	kg	1991	0.1	kg
1992	2.15	kg	1992	0.1	kg
1993	2.15	kg	1993	0.1	kg
1994	2.15	kg	1994	0.1	kg
1995	2.15	kg	1995	0.1	kg
1996	2.15	kg	1996	0.1	kg
1997	2.15	kg	1997	0.1	kg
1998	2.15	kg	1998	0.1	kg
1999	2.15	kg	1999	0.1	kg
2000	2.15	kg	2000	0.1	kg
2001	2.15	kg	2001	0.1	kg
2002	2.15	kg	2002	0.1	kg
2003	2.15	kg	2003	0.1	kg
2004	2.15	kg	2004	0.1	kg
2005	2.15	kg	2005	0.1	kg
2006	2.15	kg	2006	0.1	kg
2007	2.15	kg	2007	0.1	kg
2008	2.15	kg	2008	0.1	kg
2009	2.15	kg	2009	0.1	kg
2010	2.15	kg	2010	0.1	kg
2011	2.15	kg	2011	0.1	kg
2012	2.15	kg	2012	0.1	kg
2013	2.15	kg	2013	0.1	kg
2014	2.15	kg	2014	0.1	kg
2015	2.15	kg	2015	0.1	kg
2016	2.15	kg	2016	0.1	kg
2017	2.15	kg	2017	0.1	kg
2018	2.15	kg	2018	0.1	kg
2019	2.15	kg	2019	0.1	kg
2020	2.15	kg	2020	0.1	kg

TABLE I (Continued)

hk ℓ	Calc.	Obs.	hk ℓ	Calc.	Obs.
652	- 4.8	5.2	802	+ 9.7	9.5
662	- 0.3	0	812	+ 9.7	11.8
672	- 2.0	0	822	+11.0	8.6
682	+ 5.6	5.5	832	-10.3	10.6
692	- 2.2	0	842	+ 0.7	0
702	-22.8	21.8	852	+ 8.0	8.6
712	+ 2.2	0	862	- 0.5	0
722	- 8.9	9.2	872	- 4.6	5.2
732	- 2.0	4.3	882	- 0.1	0
742	- 7.5	6.6	902	- 1.2	0
752	+ 0.7	0	912	+ 4.1	0
762	+ 6.6	5.2	922	+ 0.7	0
772	- 4.9	4.0	932	+ 4.3	0
782	- 4.2	0	942	- 2.4	0
792	- 2.2	0	952	+ 5.7	4.3
8,10,2	- 4.1	4.9	962	- 1.3	0
8,11,2	- 2.3	0	10,3,2	- 6.4	0
702	-13.2	14.3	10,1,2	+ 7.5	0
712	- 3.2	4.6	10,2,2	- 5.8	0
722	- 1.2	0	10,3,2	- 5.8	0
732	+ 9.1	7.8	003	+25.4	31.6
742	- 8.3	8.0	013	+11.9	13.2
752	- 1.8	0	023	- 5.4	4.6
762	+ 2.6	3.7	033	-10.9	9.5
772	+ 0.7	0	043	- 2.2	2.0
702	+ 0.1	0	053	- 2.1	0
712	+ 3.0	5.7	063	-18.5	16.4
722	+ 3.9	4.6	073	-13.1	10.6
732	-16.1	16.1	083	+ 3.5	0
742	+ 1.5	0	093	- 1.1	0
752	- 1.4	0	0,10,3	+ 1.0	0
762	+ 5.1	5.7	0,11,3	- 8.1	7.8
772	- 4.0	4.6	0,12,3	+ 5.8	7.5
782	+ 0.4	0	103	-18.0	18.4
792	+ 4.7	5.4	113	-19.7	18.7
7,10,2	+ 0.2	0	123	- 5.8	5.2
802	+ 8.2	8.3	133	- 2.7	3.4
812	- 1.9	0	143	-21.7	24.1
822	- 3.5	4.6	153	-11.4	7.2
832	+ 5.9	6.6	163	- 1.7	0
842	+ 2.8	4.3	173	+14.1	8.9
852	- 0.3	0			

TABLE 2 (Continued)

Year	Value	Unit	Year	Value	Unit
1950	1.0	100	1950	1.0	100
1951	1.1	100	1951	1.1	100
1952	1.2	100	1952	1.2	100
1953	1.3	100	1953	1.3	100
1954	1.4	100	1954	1.4	100
1955	1.5	100	1955	1.5	100
1956	1.6	100	1956	1.6	100
1957	1.7	100	1957	1.7	100
1958	1.8	100	1958	1.8	100
1959	1.9	100	1959	1.9	100
1960	2.0	100	1960	2.0	100
1961	2.1	100	1961	2.1	100
1962	2.2	100	1962	2.2	100
1963	2.3	100	1963	2.3	100
1964	2.4	100	1964	2.4	100
1965	2.5	100	1965	2.5	100
1966	2.6	100	1966	2.6	100
1967	2.7	100	1967	2.7	100
1968	2.8	100	1968	2.8	100
1969	2.9	100	1969	2.9	100
1970	3.0	100	1970	3.0	100
1971	3.1	100	1971	3.1	100
1972	3.2	100	1972	3.2	100
1973	3.3	100	1973	3.3	100
1974	3.4	100	1974	3.4	100
1975	3.5	100	1975	3.5	100
1976	3.6	100	1976	3.6	100
1977	3.7	100	1977	3.7	100
1978	3.8	100	1978	3.8	100
1979	3.9	100	1979	3.9	100
1980	4.0	100	1980	4.0	100
1981	4.1	100	1981	4.1	100
1982	4.2	100	1982	4.2	100
1983	4.3	100	1983	4.3	100
1984	4.4	100	1984	4.4	100
1985	4.5	100	1985	4.5	100
1986	4.6	100	1986	4.6	100
1987	4.7	100	1987	4.7	100
1988	4.8	100	1988	4.8	100
1989	4.9	100	1989	4.9	100
1990	5.0	100	1990	5.0	100
1991	5.1	100	1991	5.1	100
1992	5.2	100	1992	5.2	100
1993	5.3	100	1993	5.3	100
1994	5.4	100	1994	5.4	100
1995	5.5	100	1995	5.5	100
1996	5.6	100	1996	5.6	100
1997	5.7	100	1997	5.7	100
1998	5.8	100	1998	5.8	100
1999	5.9	100	1999	5.9	100
2000	6.0	100	2000	6.0	100
2001	6.1	100	2001	6.1	100
2002	6.2	100	2002	6.2	100
2003	6.3	100	2003	6.3	100
2004	6.4	100	2004	6.4	100
2005	6.5	100	2005	6.5	100
2006	6.6	100	2006	6.6	100
2007	6.7	100	2007	6.7	100
2008	6.8	100	2008	6.8	100
2009	6.9	100	2009	6.9	100
2010	7.0	100	2010	7.0	100
2011	7.1	100	2011	7.1	100
2012	7.2	100	2012	7.2	100
2013	7.3	100	2013	7.3	100
2014	7.4	100	2014	7.4	100
2015	7.5	100	2015	7.5	100
2016	7.6	100	2016	7.6	100
2017	7.7	100	2017	7.7	100
2018	7.8	100	2018	7.8	100
2019	7.9	100	2019	7.9	100
2020	8.0	100	2020	8.0	100

TABLE I (Continued)

hkl	Calc.	Obs.	hkl	Calc.	Obs.
183	- 8.0	0	303	- 4.7	7.5
193	+ 1.1	0	313	+ 1.8	0
1,10,3	+ 0.4	0	323	+20.7	22.1
1,11,3	+ 3.8	0	333	+15.7	12.1
1,12,3	- 2.4	0	343	+ 2.3	4.6
$\bar{1}$ 03	+ 7.0	0	353	+ 2.2	0
$\bar{1}$ 13	- 5.6	6.0	363	+14.6	12.3
$\bar{1}$ 23	+19.8	24.4	373	- 1.4	0
$\bar{1}$ 33	+28.8	26.4	383	- 3.0	0
$\bar{1}$ 43	+11.6	11.8	393	- 6.0	0
$\bar{1}$ 53	-10.6	7.5	3,10,3	+ 6.1	0
$\bar{1}$ 63	+ 9.8	10.3	3,11,3	+ 2.0	0
$\bar{1}$ 73	+ 0.5	0	$\bar{3}$ 03	-14.8	14.9
$\bar{1}$ 83	+ 1.4	0	$\bar{3}$ 13	-23.2	21.2
$\bar{1}$ 93	-14.3	11.8	$\bar{3}$ 23	-11.5	10.3
$\bar{1}$,10,3	+ 4.9	4.6	$\bar{3}$ 33	+ 0.8	0
$\bar{1}$,11,3	+ 0.2	0	$\bar{3}$ 43	-15.5	15.2
$\bar{1}$,12,3	- 0.6	0	$\bar{3}$ 53	-11.1	7.8
203	- 7.3	4.6	$\bar{3}$ 63	- 3.2	3.7
213	+13.7	14.9	$\bar{3}$ 73	+18.4	16.4
223	-11.8	12.3	$\bar{3}$ 83	- 4.8	0
233	-13.4	16.1	$\bar{3}$ 93	+ 1.6	0
243	+11.7	12.0	$\bar{3}$,10,3	- 2.2	0
253	+19.5	17.8	$\bar{3}$,11,3	+ 6.2	6.0
263	+ 4.1	0	$\bar{3}$,12,3	- 1.6	0
273	- 2.6	0	403	+ 8.0	4.6
283	+ 4.3	0	413	+ 8.8	13.2
293	+12.0	8.3	423	+ 8.4	7.8
2,10,3	- 6.6	0	433	- 6.4	6.9
2,11,3	- 0.5	0	443	- 5.9	5.2
2,12,3	- 1.2	0	453	+ 0.3	0
$\bar{2}$ 03	-13.2	20.4	463	- 3.4	0
$\bar{2}$ 13	-11.5	12.0	473	- 9.9	8.0
$\bar{2}$ 23	- 1.9	0	483	- 1.8	0
$\bar{2}$ 33	+12.2	10.1	493	- 0.6	0
$\bar{2}$ 43	+12.7	10.1	4,10,3	+ 4.8	2.9
$\bar{2}$ 53	+ 2.2	0	$\bar{4}$ 03	+ 0.5	0
$\bar{2}$ 63	+12.5	10.1	$\bar{4}$ 13	-17.5	15.2
$\bar{2}$ 73	+12.4	9.8	$\bar{4}$ 23	+ 7.6	8.6
$\bar{2}$ 83	+ 2.2	0	$\bar{4}$ 33	+12.8	11.4
$\bar{2}$ 93	+ 0.3	0	$\bar{4}$ 43	-19.5	16.6
$\bar{2}$,10,3	- 4.2	0	$\bar{4}$ 53	-21.4	17.5
$\bar{2}$,11,3	+ 7.9	7.2	$\bar{4}$ 63	+ 6.2	0
$\bar{2}$,12,3	- 3.3	4.3	$\bar{4}$ 73	+ 6.5	0

TABLE 1 (Continued)

Year	Value	Unit	Year	Value	Unit
1970	1.4	kg	1970	1.4	kg
1971	1.4	kg	1971	1.4	kg
1972	1.4	kg	1972	1.4	kg
1973	1.4	kg	1973	1.4	kg
1974	1.4	kg	1974	1.4	kg
1975	1.4	kg	1975	1.4	kg
1976	1.4	kg	1976	1.4	kg
1977	1.4	kg	1977	1.4	kg
1978	1.4	kg	1978	1.4	kg
1979	1.4	kg	1979	1.4	kg
1980	1.4	kg	1980	1.4	kg
1981	1.4	kg	1981	1.4	kg
1982	1.4	kg	1982	1.4	kg
1983	1.4	kg	1983	1.4	kg
1984	1.4	kg	1984	1.4	kg
1985	1.4	kg	1985	1.4	kg
1986	1.4	kg	1986	1.4	kg
1987	1.4	kg	1987	1.4	kg
1988	1.4	kg	1988	1.4	kg
1989	1.4	kg	1989	1.4	kg
1990	1.4	kg	1990	1.4	kg
1991	1.4	kg	1991	1.4	kg
1992	1.4	kg	1992	1.4	kg
1993	1.4	kg	1993	1.4	kg
1994	1.4	kg	1994	1.4	kg
1995	1.4	kg	1995	1.4	kg
1996	1.4	kg	1996	1.4	kg
1997	1.4	kg	1997	1.4	kg
1998	1.4	kg	1998	1.4	kg
1999	1.4	kg	1999	1.4	kg
2000	1.4	kg	2000	1.4	kg
2001	1.4	kg	2001	1.4	kg
2002	1.4	kg	2002	1.4	kg
2003	1.4	kg	2003	1.4	kg
2004	1.4	kg	2004	1.4	kg
2005	1.4	kg	2005	1.4	kg
2006	1.4	kg	2006	1.4	kg
2007	1.4	kg	2007	1.4	kg
2008	1.4	kg	2008	1.4	kg
2009	1.4	kg	2009	1.4	kg
2010	1.4	kg	2010	1.4	kg
2011	1.4	kg	2011	1.4	kg
2012	1.4	kg	2012	1.4	kg
2013	1.4	kg	2013	1.4	kg
2014	1.4	kg	2014	1.4	kg
2015	1.4	kg	2015	1.4	kg
2016	1.4	kg	2016	1.4	kg
2017	1.4	kg	2017	1.4	kg
2018	1.4	kg	2018	1.4	kg
2019	1.4	kg	2019	1.4	kg
2020	1.4	kg	2020	1.4	kg

TABLE I (Continued)

hk ℓ	Calc.	Obs.	hk ℓ	Calc.	Obs.
$\overline{483}$	- 6.9	6.9	$\overline{653}$	- 4.6	3.2
$\overline{493}$	-11.5	7.8	$\overline{663}$	+12.5	11.8
$\overline{4,10,3}$	+ 6.4	6.3	$\overline{673}$	+11.2	10.1
$\overline{4,11,3}$	+ 1.5	0	$\overline{683}$	- 0.1	0
$\overline{4,12,3}$	+ 0.6	0	$\overline{693}$	- 4.6	0
			$\overline{6,10,3}$	- 0.5	0
503	-13.1	11.4	703	- 3.2	0
513	- 5.6	0	713	+ 1.8	3.7
523	+ 3.0	0	723	+ 7.7	6.9
533	- 5.7	0	733	+ 4.8	2.9
543	-17.0	16.6	743	+ 1.3	2.3
553	- 4.2	0	753	+ 1.8	0
563	+ 2.2	0	763	+ 6.4	0
573	+ 3.6	0			
583	- 7.3	0	$\overline{703}$	-10.4	10.6
593	+ 2.6	0	$\overline{713}$	+ 0.4	0
$\overline{503}$	+ 4.6	5.2	$\overline{723}$	- 3.3	6.0
$\overline{513}$	+ 4.5	4.3	$\overline{733}$	-10.3	9.2
$\overline{523}$	+15.2	12.4	$\overline{743}$	- 8.7	8.3
$\overline{533}$	+13.2	12.6	$\overline{753}$	+ 5.0	3.7
$\overline{543}$	+ 5.1	6.3	$\overline{763}$	+ 1.5	0
$\overline{553}$	- 4.3	0	$\overline{773}$	+ 3.5	0
$\overline{563}$	+ 6.4	0	$\overline{783}$	- 3.7	0
$\overline{573}$	- 5.7	0	$\overline{793}$	+ 7.8	6.0
$\overline{583}$	- 0.2	0			
$\overline{593}$	- 9.1	10.4	803	+ 1.1	0
$\overline{5,10,3}$	+ 4.8	0	813	- 0.3	0
$\overline{5,11,3}$	- 0.5	0			
603	-13.0	11.2	$\overline{803}$	+ 4.3	5.7
613	- 2.5	0	$\overline{813}$	- 6.8	10.3
623	+ 1.0	0	$\overline{823}$	- 3.6	0
633	+ 0.2	0	$\overline{833}$	+ 3.4	6.3
643	- 3.6	6.6	$\overline{843}$	- 6.1	0
653	+ 2.4	0	$\overline{853}$	- 8.8	10.9
663	+ 7.1	7.2	$\overline{863}$	- 8.0	7.2
673	+ 4.5	0	$\overline{873}$	+ 2.8	5.7
683	- 3.3	0	$\overline{883}$	- 0.7	0
$\overline{603}$	- 9.2	12.4	$\overline{903}$	+ 3.1	0
$\overline{613}$	-12.6	14.9	$\overline{913}$	+ 8.2	9.5
$\overline{623}$	+ 5.8	6.0	$\overline{923}$	+ 4.6	5.5
$\overline{633}$	+15.6	14.6	$\overline{933}$	- 1.9	0
$\overline{643}$	+ 7.0	4.9	$\overline{943}$	+ 1.9	0
			$\overline{953}$	+ 3.5	4.6
			$\overline{963}$	+ 0.8	0

[illegible]

TABLE I (Continued)

hk ℓ	Calc.	Obs.	hk ℓ	Calc.	Obs.
$\overline{10},0,3$	+ 1.9	0	224	- 4.3	4.9
$\overline{10},1,3$	- 2.7	0	234	- 7.0	7.8
$\overline{10},2,3$	- 1.2	0	244	+16.4	14.4
$\overline{10},3,3$	+ 4.5	0	254	- 2.5	0
004	+21.6	28.7	264	+ 4.2	5.2
014	+11.3	10.3	274	- 4.3	0
024	-10.2	8.3	284	+ 4.8	0
034	- 3.3	0	294	- 1.7	0
044	- 3.3	5.5	2,10,4	- 4.1	0
054	+12.7	9.5	$\overline{204}$	- 8.8	13.8
064	-16.8	15.5	$\overline{214}$	+11.8	11.2
074	- 1.1	0	$\overline{224}$	- 6.8	6.6
084	+ 4.4	0	$\overline{234}$	-16.4	16.4
094	+ 7.9	6.6	$\overline{244}$	+15.2	14.6
0,10,4	- 1.8	0	$\overline{254}$	+ 4.5	5.7
0,11,4	+ 0.7	0	$\overline{264}$	+ 5.4	4.9
104	+21.6	32.7	$\overline{274}$	-13.8	11.2
114	+ 1.7	0	$\overline{284}$	+ 3.3	0
124	+ 1.3	0	$\overline{294}$	+ 1.5	0
134	-17.8	18.7	$\overline{2,10,4}$	- 4.6	0
144	+14.9	15.5	$\overline{2,11,4}$	- 8.5	11.8
154	+ 9.1	5.7	304	- 5.8	0
164	- 2.5	4.9	314	+16.5	16.1
174	+ 1.9	0	324	-11.1	13.8
184	+ 8.1	0	334	- 3.2	0
194	+ 9.9	0	344	- 0.9	0
1,10,4	- 1.6	0	354	+ 6.7	6.3
1,11,4	- 0.5	0	364	- 5.2	6.0
$\overline{104}$	- 1.7	0	374	- 13.2	8.9
$\overline{114}$	+ 6.5	7.2	384	+ 0.1	0
$\overline{124}$	-23.3	23.5	394	+ 2.2	0
$\overline{134}$	+13.8	14.9	3,10,4	- 3.4	0
$\overline{144}$	+ 0.6	0	$\overline{304}$	+15.4	19.8
$\overline{154}$	- 2.8	0	$\overline{314}$	-20.7	18.4
$\overline{164}$	+13.5	11.5	$\overline{324}$	+ 8.5	6.9
$\overline{174}$	- 6.2	0	$\overline{334}$	- 1.1	3.4
$\overline{184}$	+ 2.5	0	$\overline{344}$	+12.9	10.6
$\overline{194}$	- 6.4	5.5	$\overline{354}$	- 9.1	8.6
$\overline{1,10,4}$	- 6.7	11.2	$\overline{364}$	+ 3.9	0
$\overline{1,11,4}$	- 0.9	0	$\overline{374}$	+13.8	10.6
204	- 1.2	0	$\overline{384}$	+ 5.5	5.7
214	- 0	0	$\overline{394}$	- 1.0	0
			$\overline{3,10,4}$	+ 0.7	0
			$\overline{3,11,4}$	+ 4.7	0

TABLE 1 (Continued)

Year	Age	Sex	Year	Age	Sex
1948	1.0	M	1948	1.0	M
1949	1.0	M	1949	1.0	M
1950	1.0	M	1950	1.0	M
1951	1.0	M	1951	1.0	M
1952	1.0	M	1952	1.0	M
1953	1.0	M	1953	1.0	M
1954	1.0	M	1954	1.0	M
1955	1.0	M	1955	1.0	M
1956	1.0	M	1956	1.0	M
1957	1.0	M	1957	1.0	M
1958	1.0	M	1958	1.0	M
1959	1.0	M	1959	1.0	M
1960	1.0	M	1960	1.0	M
1961	1.0	M	1961	1.0	M
1962	1.0	M	1962	1.0	M
1963	1.0	M	1963	1.0	M
1964	1.0	M	1964	1.0	M
1965	1.0	M	1965	1.0	M
1966	1.0	M	1966	1.0	M
1967	1.0	M	1967	1.0	M
1968	1.0	M	1968	1.0	M
1969	1.0	M	1969	1.0	M
1970	1.0	M	1970	1.0	M
1971	1.0	M	1971	1.0	M
1972	1.0	M	1972	1.0	M
1973	1.0	M	1973	1.0	M
1974	1.0	M	1974	1.0	M
1975	1.0	M	1975	1.0	M
1976	1.0	M	1976	1.0	M
1977	1.0	M	1977	1.0	M
1978	1.0	M	1978	1.0	M
1979	1.0	M	1979	1.0	M
1980	1.0	M	1980	1.0	M
1981	1.0	M	1981	1.0	M
1982	1.0	M	1982	1.0	M
1983	1.0	M	1983	1.0	M
1984	1.0	M	1984	1.0	M
1985	1.0	M	1985	1.0	M
1986	1.0	M	1986	1.0	M
1987	1.0	M	1987	1.0	M
1988	1.0	M	1988	1.0	M
1989	1.0	M	1989	1.0	M
1990	1.0	M	1990	1.0	M
1991	1.0	M	1991	1.0	M
1992	1.0	M	1992	1.0	M
1993	1.0	M	1993	1.0	M
1994	1.0	M	1994	1.0	M
1995	1.0	M	1995	1.0	M
1996	1.0	M	1996	1.0	M
1997	1.0	M	1997	1.0	M
1998	1.0	M	1998	1.0	M
1999	1.0	M	1999	1.0	M
2000	1.0	M	2000	1.0	M

TABLE I (Continued)

hk ℓ	Calc.	Obs.	hk ℓ	Calc.	Obs.
404	+ 2.0	0	604	- 5.4	5.7
414	+ 0.7	0	614	- 4.6	4.6
424	- 0.1	0	624	+ 5.3	5.2
434	+ 5.2	5.2	634	+ 0.2	0
444	-10.6	8.9	644	+ 2.9	2.9
454	+ 1.7	0	654	- 4.1	0
464	- 5.1	0			
474	+ 2.5	0	$\bar{6}04$	-19.8	21.5
484	- 2.5	0	$\bar{6}14$	+ 9.6	10.6
494	+ 1.0	0	$\bar{6}24$	+ 3.4	0
			$\bar{6}34$	-10.0	10.0
$\bar{4}04$	+ 8.7	13.5	$\bar{6}44$	- 1.2	0
$\bar{4}14$	+13.5	14.9	$\bar{6}54$	+ 3.2	0
$\bar{4}24$	+ 8.1	4.9	$\bar{6}64$	+10.2	8.0
$\bar{4}34$	- 9.3	9.8	$\bar{6}74$	-10.7	10.3
$\bar{4}44$	-12.8	10.0	$\bar{6}84$	- 4.6	0
$\bar{4}54$	+15.9	12.4	$\bar{6}94$	+ 8.0	0
$\bar{4}64$	- 3.3	0	$\bar{6},10,4$	+ 0.8	0
$\bar{4}74$	- 2.8	0			
$\bar{4}84$	- 2.9	0	704	- 1.1	0
$\bar{4}94$	+10.7	13.5	714	+ 4.0	0
$\bar{4},10,4$	+ 4.8	0			
$\bar{4},11,4$	- 0.7	0	$\bar{7}04$	+ 2.7	0
			$\bar{7}14$	- 4.1	4.6
504	+ 8.6	0	$\bar{7}24$	+ 9.1	6.3
514	+ 2.3	0	$\bar{7}34$	- 9.0	8.0
524	+ 2.4	0	$\bar{7}44$	+ 4.5	5.2
534	- 9.8	8.0	$\bar{7}54$	- 0.1	0
544	+ 3.8	0	$\bar{7}64$	+ 6.4	0
554	+ 6.6	5.5	$\bar{7}74$	+ 2.1	0
564	- 0.6	0	$\bar{7}84$	+ 0.7	0
574	+ 0.9	0	$\bar{7}94$	+ 2.4	0
$\bar{5}04$	-12.2	11.5	$\bar{8}04$	+ 4.9	0
$\bar{5}14$	- 0.3	0	$\bar{8}14$	+ 4.9	5.4
$\bar{5}24$	- 6.4	6.3	$\bar{8}24$	+ 7.3	8.0
$\bar{5}34$	+17.5	14.6	$\bar{8}34$	- 6.2	6.3
$\bar{5}44$	-12.2	8.0	$\bar{8}44$	- 6.3	9.5
$\bar{5}54$	- 5.4	0	$\bar{8}54$	+ 4.9	6.9
$\bar{5}64$	- 3.1	0	$\bar{8}64$	+ 0.3	0
$\bar{5}74$	+ 0.1	0	$\bar{8}74$	- 2.7	0
$\bar{5}84$	- 5.1	0			
$\bar{5}94$	- 6.8	0	$\bar{9}04$	- 3.2	0
$\bar{5},10,4$	+ 0.1	0	$\bar{9}14$	+ 7.8	10.9

(continued) 1944

1940	1941	1942	1943	1944	1945
5.2	5.3 +	ACB	0	0.2 +	ACB
5.4	5.4 +	ACB	0	7.0 +	ACB
5.5	5.5 +	ACB	0	1.0 +	ACB
0	5.0 +	ACB	2.0	5.2 +	ACB
5.6	5.6 +	ACB	7.8	5.01-	ACB
0	1.4 +	ACB	0	7.1 +	ACB
			0	1.2 +	ACB
5.12	5.01-	ACB	0	5.2 +	ACB
4.01	5.2 +	ACB	0	5.2 +	ACB
0	4.2 +	ACB	0	0.1 +	ACB
0.01	5.01-	ACB			
0	2.1 +	ACB	5.01	7.8 +	ACB
0	2.2 +	ACB	7.01	5.01+	ACB
0.2	7.01+	ACB	7.2	1.0 +	ACB
5.01	7.01-	ACB	8.7	5.7 +	ACB
0	5.4 +	ACB	0.01	5.01-	ACB
0	0.8 +	ACB	4.01	7.01+	ACB
0	5.0 +	5,01,3	0	5.2 +	ACB
			0	5.0 +	ACB
0	1.1 +	ACB	0	7.2 +	ACB
0	0.4 +	ACB	5.01	7.01+	ACB
0	7.0 +	ACB	0	5.2 +	5,01,3
5.4	1.4 +	ACB	0	7.0 +	5,11,3
5.0	1.0 +	ACB	0	5.2 +	ACB
5.0	0.8 +	ACB	0	5.2 +	ACB
5.0	5.4 +	ACB	0	5.2 +	ACB
0	1.0 +	ACB	0.8	5.2 +	ACB
0	5.0 +	ACB	0	5.2 +	ACB
0	1.2 +	ACB	5.0	5.2 +	ACB
0	7.0 +	ACB	0	5.0 +	ACB
0	5.2 +	ACB	0	7.0 +	ACB
0	5.2 +	ACB	5.11	5.01-	ACB
5.0	5.2 +	ACB	0	5.0 +	ACB
5.0	5.2 +	ACB	5.0	5.2 +	ACB
5.0	5.2 +	ACB	5.41	5.01+	ACB
5.0	5.2 +	ACB	0.8	5.01-	ACB
0	5.0 +	ACB	0	5.2 +	ACB
0	5.0 +	ACB	0	1.2 +	ACB
0	5.0 +	ACB	0	1.2 +	ACB
0	5.0 +	ACB	0	5.2 +	ACB
5.0	5.2 +	ACB	0	1.0 +	5,01,3

TABLE I (Continued)

hkl	Calc.	Obs.	hkl	Calc.	Obs.
$\overline{9}24$	- 3.4	0	205	-16.0	16.3
$\overline{9}34$	+ 1.1	0	215	- 4.7	0
$\overline{9}44$	- 4.7	0	225	- 6.8	6.0
$\overline{9}54$	+ 4.4	5.7	235	+ 5.5	0
			245	- 2.8	0
$\overline{10},0,4$	- 5.5	6.3	255	- 4.5	3.7
$\overline{10},1,4$	+ 2.3	0	265	+ 3.3	0
$\overline{10},2,4$	- 3.4	0	275		NP
			285		NP
005	+20.9	30.1	295		NP
015	-14.2	12.6			
025	+ 5.5	4.9	$\overline{2}05$	- 7.4	11.2
035	+10.0	9.2	$\overline{2}15$	-13.7	12.6
045	+ 4.5	5.2	$\overline{2}25$	-18.0	14.6
055	-10.7	11.5	$\overline{2}35$	+17.6	13.5
065	- 6.2	5.2	$\overline{2}45$	+ 7.6	4.6
075		NP	$\overline{2}55$	-11.5	0
085		NP	$\overline{2}65$	- 2.3	0
095		NP	$\overline{2}75$		NP
0,10,5		NP	$\overline{2}85$		NP
			$\overline{2}95$		NP
105	- 5.3	0	$\overline{2},10,5$		NP
115	+ 0.2	0			
125	- 3.9	0	305	- 1.0	0
135	-14.7	13.2	315	+ 7.6	7.5
145	- 3.1	4.6	325	+ 4.8	7.5
155	- 0.6	0	335	+ 4.4	0
165	- 5.1	5.2	345	- 1.0	0
175		NP	355	+ 6.4	5.7
185		NP	365	+ 6.1	7.7
195		NP	375		NP
1,10,5		NP	385		NP
$\overline{1}05$	+ 8.9	9.7	$\overline{3}05$	-12.3	18.1
$\overline{1}15$	+ 6.4	6.0	$\overline{3}15$	- 8.6	6.0
$\overline{1}25$	+ 5.1	0	$\overline{3}25$	- 4.8	0
$\overline{1}35$	+10.3	8.3	$\overline{3}35$	- 7.4	6.0
$\overline{1}45$	+ 4.8	3.7	$\overline{3}45$	- 6.5	6.0
$\overline{1}55$	+ 6.1	4.6	$\overline{3}55$	- 7.6	0
$\overline{1}65$	+ 5.3	6.0	$\overline{3}65$	- 3.9	0
$\overline{1}75$		NP	$\overline{3}75$		NP
$\overline{1}85$		NP	$\overline{3}85$		NP
$\overline{1}95$		NP	$\overline{3}95$		NP
$\overline{1},10,5$		NP	$\overline{3},10,5$		NP

1995年12月15日

Year	Age	Sex	Weight	Length	Wing
1911	0.11	M	100	100	100
1912	0.12	F	100	100	100
1913	0.13	M	100	100	100
1914	0.14	F	100	100	100
1915	0.15	M	100	100	100
1916	0.16	F	100	100	100
1917	0.17	M	100	100	100
1918	0.18	F	100	100	100
1919	0.19	M	100	100	100
1920	0.20	F	100	100	100
1921	0.21	M	100	100	100
1922	0.22	F	100	100	100
1923	0.23	M	100	100	100
1924	0.24	F	100	100	100
1925	0.25	M	100	100	100
1926	0.26	F	100	100	100
1927	0.27	M	100	100	100
1928	0.28	F	100	100	100
1929	0.29	M	100	100	100
1930	0.30	F	100	100	100
1931	0.31	M	100	100	100
1932	0.32	F	100	100	100
1933	0.33	M	100	100	100
1934	0.34	F	100	100	100
1935	0.35	M	100	100	100
1936	0.36	F	100	100	100
1937	0.37	M	100	100	100
1938	0.38	F	100	100	100
1939	0.39	M	100	100	100
1940	0.40	F	100	100	100
1941	0.41	M	100	100	100
1942	0.42	F	100	100	100
1943	0.43	M	100	100	100
1944	0.44	F	100	100	100
1945	0.45	M	100	100	100
1946	0.46	F	100	100	100
1947	0.47	M	100	100	100
1948	0.48	F	100	100	100
1949	0.49	M	100	100	100
1950	0.50	F	100	100	100
1951	0.51	M	100	100	100
1952	0.52	F	100	100	100
1953	0.53	M	100	100	100
1954	0.54	F	100	100	100
1955	0.55	M	100	100	100
1956	0.56	F	100	100	100
1957	0.57	M	100	100	100
1958	0.58	F	100	100	100
1959	0.59	M	100	100	100
1960	0.60	F	100	100	100
1961	0.61	M	100	100	100
1962	0.62	F	100	100	100
1963	0.63	M	100	100	100
1964	0.64	F	100	100	100
1965	0.65	M	100	100	100
1966	0.66	F	100	100	100
1967	0.67	M	100	100	100
1968	0.68	F	100	100	100
1969	0.69	M	100	100	100
1970	0.70	F	100	100	100
1971	0.71	M	100	100	100
1972	0.72	F	100	100	100
1973	0.73	M	100	100	100
1974	0.74	F	100	100	100
1975	0.75	M	100	100	100
1976	0.76	F	100	100	100
1977	0.77	M	100	100	100
1978	0.78	F	100	100	100
1979	0.79	M	100	100	100
1980	0.80	F	100	100	100
1981	0.81	M	100	100	100
1982	0.82	F	100	100	100
1983	0.83	M	100	100	100
1984	0.84	F	100	100	100
1985	0.85	M	100	100	100
1986	0.86	F	100	100	100
1987	0.87	M	100	100	100
1988	0.88	F	100	100	100
1989	0.89	M	100	100	100
1990	0.90	F	100	100	100
1991	0.91	M	100	100	100
1992	0.92	F	100	100	100
1993	0.93	M	100	100	100
1994	0.94	F	100	100	100
1995	0.95	M	100	100	100
1996	0.96	F	100	100	100
1997	0.97	M	100	100	100
1998	0.98	F	100	100	100
1999	0.99	M	100	100	100
2000	1.00	F	100	100	100

TABLE I (Continued)

hk ℓ	Calc.	Obs.	hk ℓ	Calc.	Obs.
405	+ 5.8	0	705	- 8.0	0
415	- 1.0	0	715	- 7.1	0
425	+10.8	8.3	725	- 7.1	0
435	+ 1.2	0	735	- 2.3	0
445	- 2.8	0	745	- 1.8	0
455	- 0.1	0	755	- 5.6	0
465	+ 2.4	0	765	- 4.3	0
475		NP			
$\bar{4}05$	+15.3	20.6	$\bar{8}05$	+ 1.5	0
$\bar{4}15$	-14.1	11.5	$\bar{8}15$	+ 0.7	0
$\bar{4}25$	+ 6.4	6.0	$\bar{8}25$	+ 6.8	0
$\bar{4}35$	+ 7.3	5.5	$\bar{8}35$	- 5.5	0
$\bar{4}45$	+ 0.4	0	$\bar{8}45$	- 5.2	0
$\bar{4}55$	-11.0	0	$\bar{8}55$	+ 0.6	0
$\bar{4}65$	- 5.6	0	$\bar{8}65$	- 0.3	0
$\bar{4}75$		NP			
$\bar{4}85$		NP	$\bar{9}05$	+10.5	13.5
$\bar{4}95$		NP	$\bar{9}15$	- 0.6	0
$\bar{4}, 10, 5$		NP	$\bar{9}25$	- 0.1	0
			$\bar{9}35$	+ 6.3	0
505	- 5.6	9.5	$\bar{9}45$	+ 5.8	0
515	- 3.1	0			
525	+ 4.1	8.6	006	+ 0.7	0
535	- 4.9	3.7	016	+ 7.1	6.9
545	- 5.0	8.0	026	- 5.3	0
555	- 2.9	0	036	- 4.1	0
			046	- 5.5	0
$\bar{5}05$	+ 7.7	0	056	+ 5.6	0
$\bar{5}15$	0	0	066	-10.3	8.0
$\bar{5}25$	+ 9.1	6.0	076		NP
$\bar{5}35$	+12.5	8.6	086		NP
$\bar{5}45$	+ 2.2	0			
$\bar{5}55$	+ 0.5	0	106	+ 5.9	0
$\bar{5}65$	+ 6.2	0	116	+ 0.1	0
$\bar{5}75$		NP	126	- 2.2	0
$\bar{5}85$		NP	136	- 4.2	0
$\bar{5}95$		NP	146	+ 3.3	0
			156	+ 1.3	0
605	-14.3	12.9	166	- 3.3	0
615	+ 0.3	0	176		NP
625	- 0.7	0			
635	+ 5.7	4.3	I06	- 0.7	0
645	- 2.6	0	I16	+ 3.7	0
655	+ 0.2	0	I26	- 5.3	0
665	+ 7.5	0	I36	+ 1.8	0
			I46	+ 1.5	0

TABLE 1 (Continued)

Row	Col 1	Col 2	Col 3	Col 4	Col 5
0	0.0	0.0	0.0	0.0	0.0
0	0.1	0.1	0.1	0.1	0.1
0	0.1	0.1	0.1	0.1	0.1
0	0.2	0.2	0.2	0.2	0.2
0	0.1	0.1	0.1	0.1	0.1
0	0.2	0.2	0.2	0.2	0.2
0	0.3	0.3	0.3	0.3	0.3
0	0.4	0.4	0.4	0.4	0.4
0	0.5	0.5	0.5	0.5	0.5
0	0.6	0.6	0.6	0.6	0.6
0	0.7	0.7	0.7	0.7	0.7
0	0.8	0.8	0.8	0.8	0.8
0	0.9	0.9	0.9	0.9	0.9
0	1.0	1.0	1.0	1.0	1.0
0	1.1	1.1	1.1	1.1	1.1
0	1.2	1.2	1.2	1.2	1.2
0	1.3	1.3	1.3	1.3	1.3
0	1.4	1.4	1.4	1.4	1.4
0	1.5	1.5	1.5	1.5	1.5
0	1.6	1.6	1.6	1.6	1.6
0	1.7	1.7	1.7	1.7	1.7
0	1.8	1.8	1.8	1.8	1.8
0	1.9	1.9	1.9	1.9	1.9
0	2.0	2.0	2.0	2.0	2.0
0	2.1	2.1	2.1	2.1	2.1
0	2.2	2.2	2.2	2.2	2.2
0	2.3	2.3	2.3	2.3	2.3
0	2.4	2.4	2.4	2.4	2.4
0	2.5	2.5	2.5	2.5	2.5
0	2.6	2.6	2.6	2.6	2.6
0	2.7	2.7	2.7	2.7	2.7
0	2.8	2.8	2.8	2.8	2.8
0	2.9	2.9	2.9	2.9	2.9
0	3.0	3.0	3.0	3.0	3.0
0	3.1	3.1	3.1	3.1	3.1
0	3.2	3.2	3.2	3.2	3.2
0	3.3	3.3	3.3	3.3	3.3
0	3.4	3.4	3.4	3.4	3.4
0	3.5	3.5	3.5	3.5	3.5
0	3.6	3.6	3.6	3.6	3.6
0	3.7	3.7	3.7	3.7	3.7
0	3.8	3.8	3.8	3.8	3.8
0	3.9	3.9	3.9	3.9	3.9
0	4.0	4.0	4.0	4.0	4.0
0	4.1	4.1	4.1	4.1	4.1
0	4.2	4.2	4.2	4.2	4.2
0	4.3	4.3	4.3	4.3	4.3
0	4.4	4.4	4.4	4.4	4.4
0	4.5	4.5	4.5	4.5	4.5
0	4.6	4.6	4.6	4.6	4.6
0	4.7	4.7	4.7	4.7	4.7
0	4.8	4.8	4.8	4.8	4.8
0	4.9	4.9	4.9	4.9	4.9
0	5.0	5.0	5.0	5.0	5.0
0	5.1	5.1	5.1	5.1	5.1
0	5.2	5.2	5.2	5.2	5.2
0	5.3	5.3	5.3	5.3	5.3
0	5.4	5.4	5.4	5.4	5.4
0	5.5	5.5	5.5	5.5	5.5
0	5.6	5.6	5.6	5.6	5.6
0	5.7	5.7	5.7	5.7	5.7
0	5.8	5.8	5.8	5.8	5.8
0	5.9	5.9	5.9	5.9	5.9
0	6.0	6.0	6.0	6.0	6.0
0	6.1	6.1	6.1	6.1	6.1
0	6.2	6.2	6.2	6.2	6.2
0	6.3	6.3	6.3	6.3	6.3
0	6.4	6.4	6.4	6.4	6.4
0	6.5	6.5	6.5	6.5	6.5
0	6.6	6.6	6.6	6.6	6.6
0	6.7	6.7	6.7	6.7	6.7
0	6.8	6.8	6.8	6.8	6.8
0	6.9	6.9	6.9	6.9	6.9
0	7.0	7.0	7.0	7.0	7.0
0	7.1	7.1	7.1	7.1	7.1
0	7.2	7.2	7.2	7.2	7.2
0	7.3	7.3	7.3	7.3	7.3
0	7.4	7.4	7.4	7.4	7.4
0	7.5	7.5	7.5	7.5	7.5
0	7.6	7.6	7.6	7.6	7.6
0	7.7	7.7	7.7	7.7	7.7
0	7.8	7.8	7.8	7.8	7.8
0	7.9	7.9	7.9	7.9	7.9
0	8.0	8.0	8.0	8.0	8.0
0	8.1	8.1	8.1	8.1	8.1
0	8.2	8.2	8.2	8.2	8.2
0	8.3	8.3	8.3	8.3	8.3
0	8.4	8.4	8.4	8.4	8.4
0	8.5	8.5	8.5	8.5	8.5
0	8.6	8.6	8.6	8.6	8.6
0	8.7	8.7	8.7	8.7	8.7
0	8.8	8.8	8.8	8.8	8.8
0	8.9	8.9	8.9	8.9	8.9
0	9.0	9.0	9.0	9.0	9.0
0	9.1	9.1	9.1	9.1	9.1
0	9.2	9.2	9.2	9.2	9.2
0	9.3	9.3	9.3	9.3	9.3
0	9.4	9.4	9.4	9.4	9.4
0	9.5	9.5	9.5	9.5	9.5
0	9.6	9.6	9.6	9.6	9.6
0	9.7	9.7	9.7	9.7	9.7
0	9.8	9.8	9.8	9.8	9.8
0	9.9	9.9	9.9	9.9	9.9
0	10.0	10.0	10.0	10.0	10.0

TABLE I (Continued)

hkl	Calc.	Obs.	hkl	Calc.	Obs.
$\overline{1}56$	+ 1.5	0	$\overline{4}06$	+ 1.3	0
$\overline{1}66$	- 2.7	0	$\overline{4}16$	- 2.5	4.9
$\overline{1}76$		NP	$\overline{4}26$	- 4.2	0
$\overline{1}86$		NP	$\overline{4}36$	+ 4.6	2.9
			$\overline{4}46$	- 5.7	0
206	+ 0.8	0	$\overline{4}56$	- 1.4	0
216	+ 9.5	6.6	$\overline{4}66$	-10.0	5.2
226	+ 3.1	0	$\overline{4}76$		NP
236	-10.9	8.9	$\overline{4}86$		NP
246	+ 5.7	4.6	$\overline{4}96$		NP
256	+ 8.0	5.5			
266	+ 7.7	5.2	$\overline{5}06$	-12.2	16.6
$\overline{2}06$	+ 4.0	0	$\overline{5}16$	+ 5.1	5.5
$\overline{2}16$	- 2.9	0	$\overline{5}26$	+ 4.3	0
$\overline{2}26$	+ 0.3	0	$\overline{5}36$	+ 0.6	0
$\overline{2}36$	+ 0.1	0	$\overline{5}46$	- 9.3	0
$\overline{2}46$	+10.5	8.6	$\overline{5}56$	+ 2.8	0
$\overline{2}56$	- 2.7	0	$\overline{5}66$	+ 3.3	0
$\overline{2}66$	+ 7.4	0	$\overline{5}76$		NP
$\overline{2}76$		NP	$\overline{5}86$		NP
$\overline{2}86$		NP			
$\overline{2}96$		NP	$\overline{6}06$	+ 0.9	0
			$\overline{6}16$	- 0.1	0
306	+ 1.2	0	$\overline{6}26$	+ 0.4	0
316	+ 0.9	0	$\overline{6}36$	- 1.5	0
326	- 3.1	0	$\overline{6}46$	+ 6.4	3.7
336	+ 2.1	0	$\overline{6}56$	- 0.7	0
346	+ 3.2	3.2	$\overline{6}66$	+ 6.3	0
356	+ 0.1	0			
$\overline{3}06$	+ 2.1	0	$\overline{7}06$	- 5.5	0
$\overline{3}16$	+ 0.3	0	$\overline{7}16$	+ 3.0	0
$\overline{3}26$	+ 5.2	0	$\overline{7}26$	+10.9	4.6
$\overline{3}46$	+ 6.0	5.2	$\overline{7}36$	- 7.3	0
$\overline{3}56$	- 0.2	0	$\overline{7}46$	- 4.5	0
$\overline{3}66$	+ 1.6	0	$\overline{7}56$	+ 3.5	0
$\overline{3}76$	+ 3.2	0	$\overline{7}66$	+ 8.8	0
$\overline{3}86$		NP			
$\overline{3}96$		NP	$\overline{8}06$	+ 1.2	0
			$\overline{8}16$	+ 1.7	0
406	- 2.6	0	$\overline{8}26$	- 1.2	0
416	+ 7.4	8.9	$\overline{8}36$	- 0.5	0
426	- 0.7	0	$\overline{8}46$	- 3.2	0
436		NP			
			007	+ 8.6	7.5
			017	+ 1.9	0

TABLE 2 (Continued)

Age	Calc.	Obs.	Age	Calc.	Obs.
100	+ 1.2	0	100	+ 1.2	0
101	- 2.7	0	101	- 2.7	0
102		0	102		0
103		0	103		0
104		0	104		0
105		0	105		0
106	+ 0.0	0	106	+ 0.0	0
107	+ 0.0	0	107	+ 0.0	0
108	+ 0.0	0	108	+ 0.0	0
109	+ 0.0	0	109	+ 0.0	0
110	+ 0.0	0	110	+ 0.0	0
111	+ 0.0	0	111	+ 0.0	0
112	+ 0.0	0	112	+ 0.0	0
113	+ 0.0	0	113	+ 0.0	0
114	+ 0.0	0	114	+ 0.0	0
115	+ 0.0	0	115	+ 0.0	0
116	+ 0.0	0	116	+ 0.0	0
117	+ 0.0	0	117	+ 0.0	0
118	+ 0.0	0	118	+ 0.0	0
119	+ 0.0	0	119	+ 0.0	0
120	+ 0.0	0	120	+ 0.0	0
121	+ 0.0	0	121	+ 0.0	0
122	+ 0.0	0	122	+ 0.0	0
123	+ 0.0	0	123	+ 0.0	0
124	+ 0.0	0	124	+ 0.0	0
125	+ 0.0	0	125	+ 0.0	0
126	+ 0.0	0	126	+ 0.0	0
127	+ 0.0	0	127	+ 0.0	0
128	+ 0.0	0	128	+ 0.0	0
129	+ 0.0	0	129	+ 0.0	0
130	+ 0.0	0	130	+ 0.0	0
131	+ 0.0	0	131	+ 0.0	0
132	+ 0.0	0	132	+ 0.0	0
133	+ 0.0	0	133	+ 0.0	0
134	+ 0.0	0	134	+ 0.0	0
135	+ 0.0	0	135	+ 0.0	0
136	+ 0.0	0	136	+ 0.0	0
137	+ 0.0	0	137	+ 0.0	0
138	+ 0.0	0	138	+ 0.0	0
139	+ 0.0	0	139	+ 0.0	0
140	+ 0.0	0	140	+ 0.0	0
141	+ 0.0	0	141	+ 0.0	0
142	+ 0.0	0	142	+ 0.0	0
143	+ 0.0	0	143	+ 0.0	0
144	+ 0.0	0	144	+ 0.0	0
145	+ 0.0	0	145	+ 0.0	0
146	+ 0.0	0	146	+ 0.0	0
147	+ 0.0	0	147	+ 0.0	0
148	+ 0.0	0	148	+ 0.0	0
149	+ 0.0	0	149	+ 0.0	0
150	+ 0.0	0	150	+ 0.0	0
151	+ 0.0	0	151	+ 0.0	0
152	+ 0.0	0	152	+ 0.0	0
153	+ 0.0	0	153	+ 0.0	0
154	+ 0.0	0	154	+ 0.0	0
155	+ 0.0	0	155	+ 0.0	0
156	+ 0.0	0	156	+ 0.0	0
157	+ 0.0	0	157	+ 0.0	0
158	+ 0.0	0	158	+ 0.0	0
159	+ 0.0	0	159	+ 0.0	0
160	+ 0.0	0	160	+ 0.0	0
161	+ 0.0	0	161	+ 0.0	0
162	+ 0.0	0	162	+ 0.0	0
163	+ 0.0	0	163	+ 0.0	0
164	+ 0.0	0	164	+ 0.0	0
165	+ 0.0	0	165	+ 0.0	0
166	+ 0.0	0	166	+ 0.0	0
167	+ 0.0	0	167	+ 0.0	0
168	+ 0.0	0	168	+ 0.0	0
169	+ 0.0	0	169	+ 0.0	0
170	+ 0.0	0	170	+ 0.0	0
171	+ 0.0	0	171	+ 0.0	0
172	+ 0.0	0	172	+ 0.0	0
173	+ 0.0	0	173	+ 0.0	0
174	+ 0.0	0	174	+ 0.0	0
175	+ 0.0	0	175	+ 0.0	0
176	+ 0.0	0	176	+ 0.0	0
177	+ 0.0	0	177	+ 0.0	0
178	+ 0.0	0	178	+ 0.0	0
179	+ 0.0	0	179	+ 0.0	0
180	+ 0.0	0	180	+ 0.0	0
181	+ 0.0	0	181	+ 0.0	0
182	+ 0.0	0	182	+ 0.0	0
183	+ 0.0	0	183	+ 0.0	0
184	+ 0.0	0	184	+ 0.0	0
185	+ 0.0	0	185	+ 0.0	0
186	+ 0.0	0	186	+ 0.0	0
187	+ 0.0	0	187	+ 0.0	0
188	+ 0.0	0	188	+ 0.0	0
189	+ 0.0	0	189	+ 0.0	0
190	+ 0.0	0	190	+ 0.0	0
191	+ 0.0	0	191	+ 0.0	0
192	+ 0.0	0	192	+ 0.0	0
193	+ 0.0	0	193	+ 0.0	0
194	+ 0.0	0	194	+ 0.0	0
195	+ 0.0	0	195	+ 0.0	0
196	+ 0.0	0	196	+ 0.0	0
197	+ 0.0	0	197	+ 0.0	0
198	+ 0.0	0	198	+ 0.0	0
199	+ 0.0	0	199	+ 0.0	0
200	+ 0.0	0	200	+ 0.0	0

TABLE I (Continued)

hkl	Calc.	Obs.	hkl	Calc.	Obs.
027	+ 6.8	6.0	$\bar{4}07$	+ 7.1	9.5
037	+ 1.5	0	$\bar{4}17$	- 2.5	0
047	- 0.6	0	$\bar{4}27$	+ 9.8	5.4
057	+ 0.1	0	$\bar{4}37$	+ 3.8	0
			$\bar{4}47$	- 2.2	0
107	+ 6.4	9.8	$\bar{4}57$	- 4.0	0
117	- 4.1	0	$\bar{4}67$	+ 1.9	0
127	- 1.5	0			
137	- 4.7	3.7	507	+ 2.3	0
147	+ 2.6	0	517	- 1.0	0
			527	- 1.5	0
$\bar{1}07$	+ 4.3	0	537	+10.5	5.7
$\bar{1}17$	- 1.3	0	547	+ 2.9	0
$\bar{1}27$	- 7.7	4.3	557	- 0.8	0
$\bar{1}37$	+11.0	6.6	567	- 2.0	0
$\bar{1}47$	+ 7.3	4.9			
$\bar{1}57$	- 0.7	0	$\bar{6}07$	-10.6	11.2
$\bar{1}67$	- 5.8	0	$\bar{6}17$	- 2.8	0
			$\bar{6}27$	- 4.5	0
207	- 6.5	6.0	$\bar{6}37$	+ 2.3	0
217	- 1.3	0	$\bar{6}47$	- 1.7	0
227	- 5.3	0	$\bar{6}57$	- 0.6	0
$\bar{2}07$	-13.9	19.2	707	- 0.3	0
$\bar{2}17$	- 2.4	0	717	- 2.7	0
$\bar{2}27$	- 3.9	0	727	- 2.0	0
$\bar{2}37$	- 0.2	0	737	- 5.2	0
$\bar{2}47$	- 3.5	0			
$\bar{2}57$	- 0.2	0	$\bar{2}08$	+ 0.9	0
$\bar{2}67$	+ 3.1	0			
			$\bar{3}08$	- 3.5	0
307	+ 7.9	9.8	$\bar{3}18$	- 2.0	0
317	-10.8	9.2			
327	- 6.0	0	$\bar{4}08$	- 1.7	0
337	+ 0.3	0	$\bar{4}18$		NP
347	+ 4.2	0			
357	- 9.3	0			
367	- 4.4	0			

It is seen that general agreement is very good. Any large discrepancies may arise from poor intensity estimation

TABLE 2 (Continued)

Year	Value	Year	Value	Year	Value
1957	1.7 +	1967	1.7 +	1977	1.7 +
1958	2.2 +	1968	2.2 +	1978	2.2 +
1959	2.8 +	1969	2.8 +	1979	2.8 +
1960	3.4 +	1970	3.4 +	1980	3.4 +
1961	4.0 +	1971	4.0 +	1981	4.0 +
1962	4.6 +	1972	4.6 +	1982	4.6 +
1963	5.2 +	1973	5.2 +	1983	5.2 +
1964	5.8 +	1974	5.8 +	1984	5.8 +
1965	6.4 +	1975	6.4 +	1985	6.4 +
1966	7.0 +	1976	7.0 +	1986	7.0 +
1967	7.6 +	1977	7.6 +	1987	7.6 +
1968	8.2 +	1978	8.2 +	1988	8.2 +
1969	8.8 +	1979	8.8 +	1989	8.8 +
1970	9.4 +	1980	9.4 +	1990	9.4 +
1971	10.0 +	1981	10.0 +	1991	10.0 +
1972	10.6 +	1982	10.6 +	1992	10.6 +
1973	11.2 +	1983	11.2 +	1993	11.2 +
1974	11.8 +	1984	11.8 +	1994	11.8 +
1975	12.4 +	1985	12.4 +	1995	12.4 +
1976	13.0 +	1986	13.0 +	1996	13.0 +
1977	13.6 +	1987	13.6 +	1997	13.6 +
1978	14.2 +	1988	14.2 +	1998	14.2 +
1979	14.8 +	1989	14.8 +	1999	14.8 +
1980	15.4 +	1990	15.4 +	2000	15.4 +
1981	16.0 +	1991	16.0 +	2001	16.0 +
1982	16.6 +	1992	16.6 +	2002	16.6 +
1983	17.2 +	1993	17.2 +	2003	17.2 +
1984	17.8 +	1994	17.8 +	2004	17.8 +
1985	18.4 +	1995	18.4 +	2005	18.4 +
1986	19.0 +	1996	19.0 +	2006	19.0 +
1987	19.6 +	1997	19.6 +	2007	19.6 +
1988	20.2 +	1998	20.2 +	2008	20.2 +
1989	20.8 +	1999	20.8 +	2009	20.8 +
1990	21.4 +	2000	21.4 +	2010	21.4 +
1991	22.0 +	2001	22.0 +	2011	22.0 +
1992	22.6 +	2002	22.6 +	2012	22.6 +
1993	23.2 +	2003	23.2 +	2013	23.2 +
1994	23.8 +	2004	23.8 +	2014	23.8 +
1995	24.4 +	2005	24.4 +	2015	24.4 +
1996	25.0 +	2006	25.0 +	2016	25.0 +
1997	25.6 +	2007	25.6 +	2017	25.6 +
1998	26.2 +	2008	26.2 +	2018	26.2 +
1999	26.8 +	2009	26.8 +	2019	26.8 +
2000	27.4 +	2010	27.4 +	2020	27.4 +

It is not clear that the general agreement is very good. Any large discrepancies may arise from insufficient

and to the use of the isotropic temperature factor. The non-cylindrical cross section of the crystals used for photography increased the difficulty of good cross-calibration of intensities and may account for some errors. For the cut crystals the character of the spots left much to be desired so some deviations are to be expected for this reason. The parameters used for calculation of amplitudes were determined from observed data alone and thus final positions include no corrections for incomplete series. At high values of $(\sin \theta)/\lambda$ very small changes in coordinates have a relatively large effect on F_{calc} . and some of the differences may be resolved by better parameter values. The determination of an F calc. synthesis is now in progress but will not be reported here.

A criterion of the quality of a structure determination has been suggested by Smare⁽¹⁸⁾ and Broomhead and Nichol⁽⁴⁾ wherein an "index of reliability" is determined as

$$R = \frac{\sum | |F_{\text{obs.}}| - |F_{\text{calc.}}| |}{\sum |F_{\text{obs.}}|}.$$

Applied to the data herein two values of the index were evaluated. When only reflections for which observed data are available are considered, $R = 0.17$. If amplitudes, the calculation of which indicates they are too weak to observe (i.e. < 3), are omitted but all others are

and to the use of the logarithmic temperature factor.
The non-cylindrical cross section of the crystals used
for photography increased the difficulty of good cross-
calibration of facettations and may account for some errors.
For the cut crystals the character of the spots left

much to be desired as some deviations are to be expected
for this reason. The parameters used for calculation of
amplitudes were determined from observed data alone and
that final position includes no corrections for inhomogene-
ities. At high values of $\sin \theta/\lambda$ very small changes in
amplitudes have a relatively large effect on F_{calc} . The
some of the differences may be resolved by better parameter
values. The determination of an F_{calc} synthesis is
now in progress but will not be reported here.

A criterion of the quality of a structure determina-
tion has been suggested by ⁽¹²⁾ and ⁽¹³⁾ and ⁽¹⁴⁾ and ⁽¹⁵⁾
Michael⁽¹⁴⁾ where an "index of reliability" is determined

as

$$R = \frac{\sum |F_{obs}| - \sum |F_{calc}|}{\sum |F_{obs}|}$$

Applied to the data herein two values of the index were
evaluated. When only reflections for which observed data
are available are considered, $R = 0.17$. It includes
the calculation of which indicates they are too weak to
observe ($I < 3$), are omitted but all others are

considered, then $R = 0.21$. These values compare favorably with those obtained in other structure determinations by other investigators. More recently it has been suggested that the index is not as good an indication of the quality of a structure as originally supposed.

The quality of a structure is originally supposed.

It must be noted that the index is not as good an indication of
by other investigators. More recently it has been sug-
gested that there occurred in other structure determinations
connected, from 0.011. These values compare favor-

DISCUSSION OF THE STRUCTURE

As has been stated, there are two strings of molecules, one in the plane $y = 1/4$ and the other in $y = 3/4$ so oriented with respect to each other as to satisfy best packing relations. Distances of close approach in the cell have been calculated and are shown in Figure 9.

To simplify the discussion of the molecular structure the atoms of the molecule have been labelled in Figure 2. Figure 10 is a sketch showing distances and angles between the atoms lying in the symmetry plane. A similar sketch for the atoms occupying fourfold positions is shown in Figure 11. Table II below lists pertinent intramolecular distances and angles together with average values of interest.

TABLE II
(All Distances in Angstroms)

C ₁ - Cl ₇	1.80	Cl ₁ - Cl ₄	2.81
C ₁ - Cl ₆	1.67	Cl ₅ - Cl ₈	2.84
C ₃ - Cl ₈	1.75	Cl ₆ - Cl ₇	2.82
C ₃ - Cl ₅	1.82	Average	2.82
C ₂ - Cl ₁	1.75	Cl ₇ - Cl ₈	4.93
C ₂ - Cl ₄	1.71	Cl ₃ - Cl ₄	4.92
Average	1.75	Average	4.92

As has been stated, there are two regions of order, one in the plane $y = 1/2$ and the other in $y = 1/4$. In oriented with respect to each other as is easily seen from Figure 1. Distances of lines measured in the cell have been calculated and are shown in Figure 2. To simplify the discussion of the molecular structure the atoms of the molecule have been labeled in Figure 1. Figure 1 is a sketch showing distances and angles between the atoms lying in the symmetry plane, a similar sketch for the atoms occupying tetrahedral positions is shown in Figure 11. Table II below lists positions of atoms and angles together with average values of interest.

TABLE II
(All Distances in Angstroms)

$C_1 - C_2$	1.35	$C_1 - C_3$	1.35
$C_1 - C_4$	1.47	$C_1 - C_5$	1.35
$C_2 - C_3$	1.35	$C_2 - C_4$	1.35
$C_2 - C_5$	1.35	$C_3 - C_4$	1.35
$C_3 - C_4$	1.35	$C_3 - C_5$	1.35
$C_4 - C_5$	1.35	$C_4 - C_6$	1.35
$C_5 - C_6$	1.35	$C_5 - C_7$	1.35
$C_6 - C_7$	1.35	$C_6 - C_8$	1.35
$C_7 - C_8$	1.35	$C_7 - C_9$	1.35
$C_8 - C_9$	1.35	$C_8 - C_{10}$	1.35
$C_9 - C_{10}$	1.35	$C_9 - C_{11}$	1.35
$C_{10} - C_{11}$	1.35	$C_{10} - C_{12}$	1.35
$C_{11} - C_{12}$	1.35	$C_{11} - C_{13}$	1.35
$C_{12} - C_{13}$	1.35	$C_{12} - C_{14}$	1.35
$C_{13} - C_{14}$	1.35	$C_{13} - C_{15}$	1.35
$C_{14} - C_{15}$	1.35	$C_{14} - C_{16}$	1.35
$C_{15} - C_{16}$	1.35	$C_{15} - C_{17}$	1.35
$C_{16} - C_{17}$	1.35	$C_{16} - C_{18}$	1.35
$C_{17} - C_{18}$	1.35	$C_{17} - C_{19}$	1.35
$C_{18} - C_{19}$	1.35	$C_{18} - C_{20}$	1.35
$C_{19} - C_{20}$	1.35	$C_{19} - C_{21}$	1.35
$C_{20} - C_{21}$	1.35	$C_{20} - C_{22}$	1.35
$C_{21} - C_{22}$	1.35	$C_{21} - C_{23}$	1.35
$C_{22} - C_{23}$	1.35	$C_{22} - C_{24}$	1.35
$C_{23} - C_{24}$	1.35	$C_{23} - C_{25}$	1.35
$C_{24} - C_{25}$	1.35	$C_{24} - C_{26}$	1.35
$C_{25} - C_{26}$	1.35	$C_{25} - C_{27}$	1.35
$C_{26} - C_{27}$	1.35	$C_{26} - C_{28}$	1.35
$C_{27} - C_{28}$	1.35	$C_{27} - C_{29}$	1.35
$C_{28} - C_{29}$	1.35	$C_{28} - C_{30}$	1.35
$C_{29} - C_{30}$	1.35	$C_{29} - C_{31}$	1.35
$C_{30} - C_{31}$	1.35	$C_{30} - C_{32}$	1.35
$C_{31} - C_{32}$	1.35	$C_{31} - C_{33}$	1.35
$C_{32} - C_{33}$	1.35	$C_{32} - C_{34}$	1.35
$C_{33} - C_{34}$	1.35	$C_{33} - C_{35}$	1.35
$C_{34} - C_{35}$	1.35	$C_{34} - C_{36}$	1.35
$C_{35} - C_{36}$	1.35	$C_{35} - C_{37}$	1.35
$C_{36} - C_{37}$	1.35	$C_{36} - C_{38}$	1.35
$C_{37} - C_{38}$	1.35	$C_{37} - C_{39}$	1.35
$C_{38} - C_{39}$	1.35	$C_{38} - C_{40}$	1.35
$C_{39} - C_{40}$	1.35	$C_{39} - C_{41}$	1.35
$C_{40} - C_{41}$	1.35	$C_{40} - C_{42}$	1.35
$C_{41} - C_{42}$	1.35	$C_{41} - C_{43}$	1.35
$C_{42} - C_{43}$	1.35	$C_{42} - C_{44}$	1.35
$C_{43} - C_{44}$	1.35	$C_{43} - C_{45}$	1.35
$C_{44} - C_{45}$	1.35	$C_{44} - C_{46}$	1.35
$C_{45} - C_{46}$	1.35	$C_{45} - C_{47}$	1.35
$C_{46} - C_{47}$	1.35	$C_{46} - C_{48}$	1.35
$C_{47} - C_{48}$	1.35	$C_{47} - C_{49}$	1.35
$C_{48} - C_{49}$	1.35	$C_{48} - C_{50}$	1.35
$C_{49} - C_{50}$	1.35	$C_{49} - C_{51}$	1.35
$C_{50} - C_{51}$	1.35	$C_{50} - C_{52}$	1.35
$C_{51} - C_{52}$	1.35	$C_{51} - C_{53}$	1.35
$C_{52} - C_{53}$	1.35	$C_{52} - C_{54}$	1.35
$C_{53} - C_{54}$	1.35	$C_{53} - C_{55}$	1.35
$C_{54} - C_{55}$	1.35	$C_{54} - C_{56}$	1.35
$C_{55} - C_{56}$	1.35	$C_{55} - C_{57}$	1.35
$C_{56} - C_{57}$	1.35	$C_{56} - C_{58}$	1.35
$C_{57} - C_{58}$	1.35	$C_{57} - C_{59}$	1.35
$C_{58} - C_{59}$	1.35	$C_{58} - C_{60}$	1.35
$C_{59} - C_{60}$	1.35	$C_{59} - C_{61}$	1.35
$C_{60} - C_{61}$	1.35	$C_{60} - C_{62}$	1.35
$C_{61} - C_{62}$	1.35	$C_{61} - C_{63}$	1.35
$C_{62} - C_{63}$	1.35	$C_{62} - C_{64}$	1.35
$C_{63} - C_{64}$	1.35	$C_{63} - C_{65}$	1.35
$C_{64} - C_{65}$	1.35	$C_{64} - C_{66}$	1.35
$C_{65} - C_{66}$	1.35	$C_{65} - C_{67}$	1.35
$C_{66} - C_{67}$	1.35	$C_{66} - C_{68}$	1.35
$C_{67} - C_{68}$	1.35	$C_{67} - C_{69}$	1.35
$C_{68} - C_{69}$	1.35	$C_{68} - C_{70}$	1.35
$C_{69} - C_{70}$	1.35	$C_{69} - C_{71}$	1.35
$C_{70} - C_{71}$	1.35	$C_{70} - C_{72}$	1.35
$C_{71} - C_{72}$	1.35	$C_{71} - C_{73}$	1.35
$C_{72} - C_{73}$	1.35	$C_{72} - C_{74}$	1.35
$C_{73} - C_{74}$	1.35	$C_{73} - C_{75}$	1.35
$C_{74} - C_{75}$	1.35	$C_{74} - C_{76}$	1.35
$C_{75} - C_{76}$	1.35	$C_{75} - C_{77}$	1.35
$C_{76} - C_{77}$	1.35	$C_{76} - C_{78}$	1.35
$C_{77} - C_{78}$	1.35	$C_{77} - C_{79}$	1.35
$C_{78} - C_{79}$	1.35	$C_{78} - C_{80}$	1.35
$C_{79} - C_{80}$	1.35	$C_{79} - C_{81}$	1.35
$C_{80} - C_{81}$	1.35	$C_{80} - C_{82}$	1.35
$C_{81} - C_{82}$	1.35	$C_{81} - C_{83}$	1.35
$C_{82} - C_{83}$	1.35	$C_{82} - C_{84}$	1.35
$C_{83} - C_{84}$	1.35	$C_{83} - C_{85}$	1.35
$C_{84} - C_{85}$	1.35	$C_{84} - C_{86}$	1.35
$C_{85} - C_{86}$	1.35	$C_{85} - C_{87}$	1.35
$C_{86} - C_{87}$	1.35	$C_{86} - C_{88}$	1.35
$C_{87} - C_{88}$	1.35	$C_{87} - C_{89}$	1.35
$C_{88} - C_{89}$	1.35	$C_{88} - C_{90}$	1.35
$C_{89} - C_{90}$	1.35	$C_{89} - C_{91}$	1.35
$C_{90} - C_{91}$	1.35	$C_{90} - C_{92}$	1.35
$C_{91} - C_{92}$	1.35	$C_{91} - C_{93}$	1.35
$C_{92} - C_{93}$	1.35	$C_{92} - C_{94}$	1.35
$C_{93} - C_{94}$	1.35	$C_{93} - C_{95}$	1.35
$C_{94} - C_{95}$	1.35	$C_{94} - C_{96}$	1.35
$C_{95} - C_{96}$	1.35	$C_{95} - C_{97}$	1.35
$C_{96} - C_{97}$	1.35	$C_{96} - C_{98}$	1.35
$C_{97} - C_{98}$	1.35	$C_{97} - C_{99}$	1.35
$C_{98} - C_{99}$	1.35	$C_{98} - C_{100}$	1.35
$C_{99} - C_{100}$	1.35	$C_{99} - C_{101}$	1.35
$C_{100} - C_{101}$	1.35	$C_{100} - C_{102}$	1.35
$C_{101} - C_{102}$	1.35	$C_{101} - C_{103}$	1.35
$C_{102} - C_{103}$	1.35	$C_{102} - C_{104}$	1.35
$C_{103} - C_{104}$	1.35	$C_{103} - C_{105}$	1.35
$C_{104} - C_{105}$	1.35	$C_{104} - C_{106}$	1.35
$C_{105} - C_{106}$	1.35	$C_{105} - C_{107}$	1.35
$C_{106} - C_{107}$	1.35	$C_{106} - C_{108}$	1.35
$C_{107} - C_{108}$	1.35	$C_{107} - C_{109}$	1.35
$C_{108} - C_{109}$	1.35	$C_{108} - C_{110}$	1.35
$C_{109} - C_{110}$	1.35	$C_{109} - C_{111}$	1.35
$C_{110} - C_{111}$	1.35	$C_{110} - C_{112}$	1.35
$C_{111} - C_{112}$	1.35	$C_{111} - C_{113}$	1.35
$C_{112} - C_{113}$	1.35	$C_{112} - C_{114}$	1.35
$C_{113} - C_{114}$	1.35	$C_{113} - C_{115}$	1.35
$C_{114} - C_{115}$	1.35	$C_{114} - C_{116}$	1.35
$C_{115} - C_{116}$	1.35	$C_{115} - C_{117}$	1.35
$C_{116} - C_{117}$	1.35	$C_{116} - C_{118}$	1.35
$C_{117} - C_{118}$	1.35	$C_{117} - C_{119}$	1.35
$C_{118} - C_{119}$	1.35	$C_{118} - C_{120}$	1.35
$C_{119} - C_{120}$	1.35	$C_{119} - C_{121}$	1.35
$C_{120} - C_{121}$	1.35	$C_{120} - C_{122}$	1.35
$C_{121} - C_{122}$	1.35	$C_{121} - C_{123}$	1.35
$C_{122} - C_{123}$	1.35	$C_{122} - C_{124}$	1.35
$C_{123} - C_{124}$	1.35	$C_{123} - C_{125}$	1.35
$C_{124} - C_{125}$	1.35	$C_{124} - C_{126}$	1.35
$C_{125} - C_{126}$	1.35	$C_{125} - C_{127}$	1.35
$C_{126} - C_{127}$	1.35	$C_{126} - C_{128}$	1.35
$C_{127} - C_{128}$	1.35	$C_{127} - C_{129}$	1.35
$C_{128} - C_{129}$	1.35	$C_{128} - C_{130}$	1.35
$C_{129} - C_{130}$	1.35	$C_{129} - C_{131}$	1.35
$C_{130} - C_{131}$	1.35	$C_{130} - C_{132}$	1.35
$C_{131} - C_{132}$	1.35	$C_{131} - C_{133}$	1.35
$C_{132} - C_{133}$	1.35	$C_{132} - C_{134}$	1.35
$C_{133} - C_{134}$	1.35	$C_{133} - C_{135}$	1.35
$C_{134} - C_{135}$	1.35	$C_{134} - C_{136}$	1.35
$C_{135} - C_{136}$	1.35	$C_{135} - C_{137}$	1.35
$C_{136} - C_{137}$	1.35	$C_{136} - C_{138}$	1.35
$C_{137} - C_{138}$	1.35	$C_{137} - C_{139}$	1.35
$C_{138} - C_{139}$	1.35	$C_{138} - C_{140}$	1.35
$C_{139} - C_{140}$	1.35	$C_{139} - C_{141}$	1.35
$C_{140} - C_{141}$	1.35	$C_{140} - C_{142}$	1.35
$C_{141} - C_{142}$	1.35	$C_{141} - C_{143}$	1.35
$C_{142} - C_{143}$	1.35	$C_{142} - C_{144}$	1.35
$C_{143} - C_{144}$	1.35	$C_{143} - C_{145}$	1.35
$C_{144} - C_{145}$	1.35	$C_{144} - C_{146}$	1.35
$C_{145} - C_{146}$	1.35	$C_{145} - C_{147}$	1.35
$C_{146} - C_{147}$	1.35	$C_{146} - C_{148}$	1.35
$C_{147} - C_{148}$	1.35	$C_{147} - C_{149}$	1.35
$C_{148} - C_{149}$	1.35	$C_{148} - C_{150}$	1.35
$C_{149} - C_{150}$	1.35	$C_{149} - C_{151}$	1.35
$C_{150} - C_{151}$	1.35	$C_{150} - C_{152}$	1.35
$C_{151} - C_{152}$	1.35	$C_{151} - C_{153}$	1.35
$C_{152} - C_{153}$	1.35	$C_{152} - C_{154}$	1.35
$C_{153} - C_{154}$	1.35	$C_{153} - C_{155}$	1.35
$C_{154} - C_{155}$	1.35	$C_{154} - C_{156}$	1.35
$C_{155} - C_{156}$	1.35	$C_{155} - C_{157}$	1.35
$C_{156} - C_{157}$	1.35	$C_{156} - C_{158}$	1.35
$C_{157} - C_{158}$	1.35	$C_{157} - C_{159}$	1.35
$C_{158} - C_{159}$	1.35	$C_{158} - C_{160}$	1.35
$C_{159} - C_{160}$	1.35	$C_{159} - C_{161}$	1.35
$C_{160} - C_{161}$	1.35	$C_{160} - C_{162}$	1.35
$C_{161} - C_{162}$	1.35	$C_{161} - C_{163}$	1.35
$C_{162} - C_{163}$	1.35	$C_{162} - C_{164}$	1.35
$C_{163} - C_{164}$	1.35	$C_{163} - C_{165}$	1.35
$C_{164} - C_{165}$	1.35	$C_{164} - C_{166}$	1.35
$C_{165} - C_{166}$	1.35	$C_{165} - C_{167}$	1.35
$C_{166} - C_{167}$	1.35	$C_{166} - C_{168}$	1.35
$C_{167} - C_{168}$	1.35	$C_{167} - C_{169}$	1.35
$C_{168} - C_{169}$	1.35	$C_{168} - C_{170}$	1.35
$C_{169} - C_{170}$	1.35	$C_{169} - C_{171}$	1.35
$C_{170} - C_{171}$	1.35	$C_{170} - C_{172}$	1.35
$C_{171} - C_{172}$	1.35	$C_{171} - C_{173}$	1.35
$C_{172} - C_{173}$	1.35	$C_{172} - C_{174}$	1.35
$C_{173} - C_{174}$	1.35	$C_{173} - C_{175}$	1.35
$C_{174} - C_{175}$	1.35	$C_{174} - C_{176}$	1.35
$C_{175} - C_{176}$	1.35	$C_{175} - C_{177}$	1.35
$C_{176} - C_{177}$	1.35	$C_{176} - C_{178}$	1.35
$C_{177} - C_{178}$	1.35	$C_{177} - C_{179}$	1.35
$C_{178} - C_{179}$	1.35	$C_{178} - C_{180}$	1.35
$C_{179} - C_{180}$	1.35	$C_{179} - C_{181}$	1.35
$C_{180} - C_{181}$	1.35	$C_{180} - C_{182}$	1.35
$C_{181} - C_{182}$	1.35	$C_{181} - C_{183}$	1.35
$C_{182} - C_{183}$	1.35	$C_{182} - C_{184}$	1.35
$C_{183} - C_{184}$	1.35	$C_{183} - C_{185}$	1.35
$C_{184} - C_{185}$	1.35	$C_{184} - C_{186}$	1.35
$C_{185} - C_{186}$	1.35	$C_{185} - C_{187}$	1.35
$C_{186} - C_{187}$	1.35	$C_{186} - C_{188}$	1.35
$C_{187} - C_{188}$	1.35	$C_{187} - C_{189}$	1.35
$C_{188} - C_{189}$	1.35	$C_{188} - C_{190}$	1.35
$C_{189} - C_{190}$	1.35	$C_{189} - C_{191}$	1.35
$C_{190} - C_{191}$	1.35	$C_{190} - C_{192}$	1.35
$C_{191} - C_{192}$	1.35	$C_{191} - C_{193}$	1.35
$C_{192} - C_{193}$	1.35	$C_{192} - C_{194}$	1.35
$C_{193} - C_{194}$	1.35	$C_{193} - C_{195}$	1.35
$C_{194} - C_{195}$	1.35	$C_{194} - C_{196}$	1.

TABLE II (Continued)

Cl ₅ - Cl ₆	3.36	Cl ₄ - Cl ₇	3.96
Cl ₁ - Cl ₂	3.38	Cl ₄ - Cl ₈	4.00
Average	3.37	Average	3.98
C ₁ - C ₃	2.12	∠ Cl ₁ -C ₂ -C ₄	108° - 20'
C ₂ - C ₄	2.21	∠ Cl ₆ -C ₁ -Cl ₇	108° - 20'
Average	2.16	∠ Cl ₅ -C ₃ -Cl ₈	106°
		Average	107° - 33'
C ₁ - C ₂	1.59		
C ₃ - C ₂	1.55	∠ C ₁ -C ₂ -C ₃	85°
Average	1.57	∠ C ₂ -C ₁ -C ₄	88°
		Average	86° .5
Cl ₄ - Cl ₆	3.06		
Cl ₄ - Cl ₅	3.10		
Cl ₁ - Cl ₇	3.11		
Cl ₁ - Cl ₈	3.07		
Average	3.08		

The twofold chlorine atoms form an isosceles trapezoid lying in the symmetry plane and the chlorines occupying fourfold positions form a similar trapezoid essentially of the same dimensions which lies almost in the plane $x = 1/4$. The two trapezoids are so oriented as to give the idealized molecule the symmetry $\bar{4}m$. From an inspection of the Cl - Cl separations on each side of

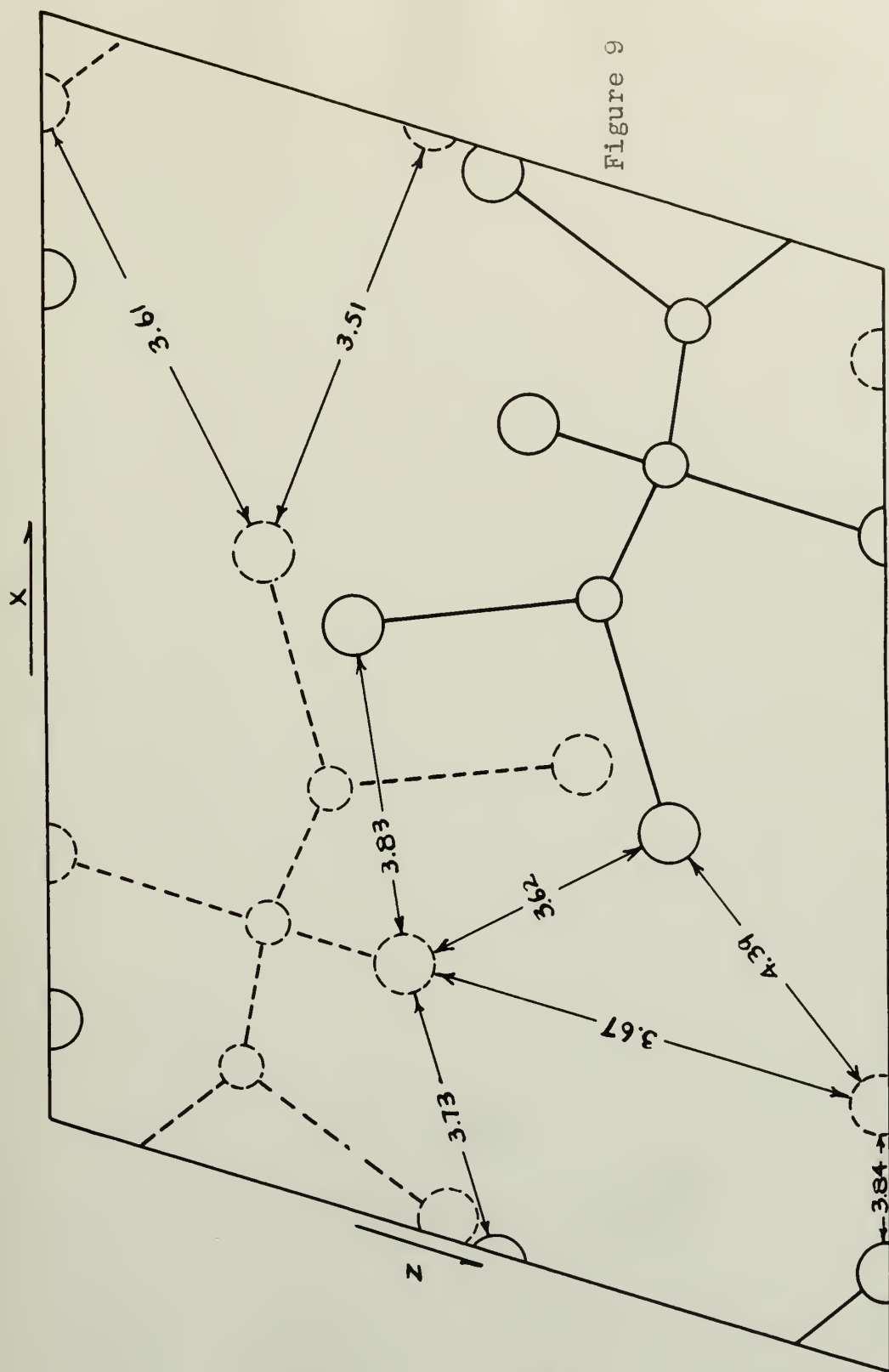
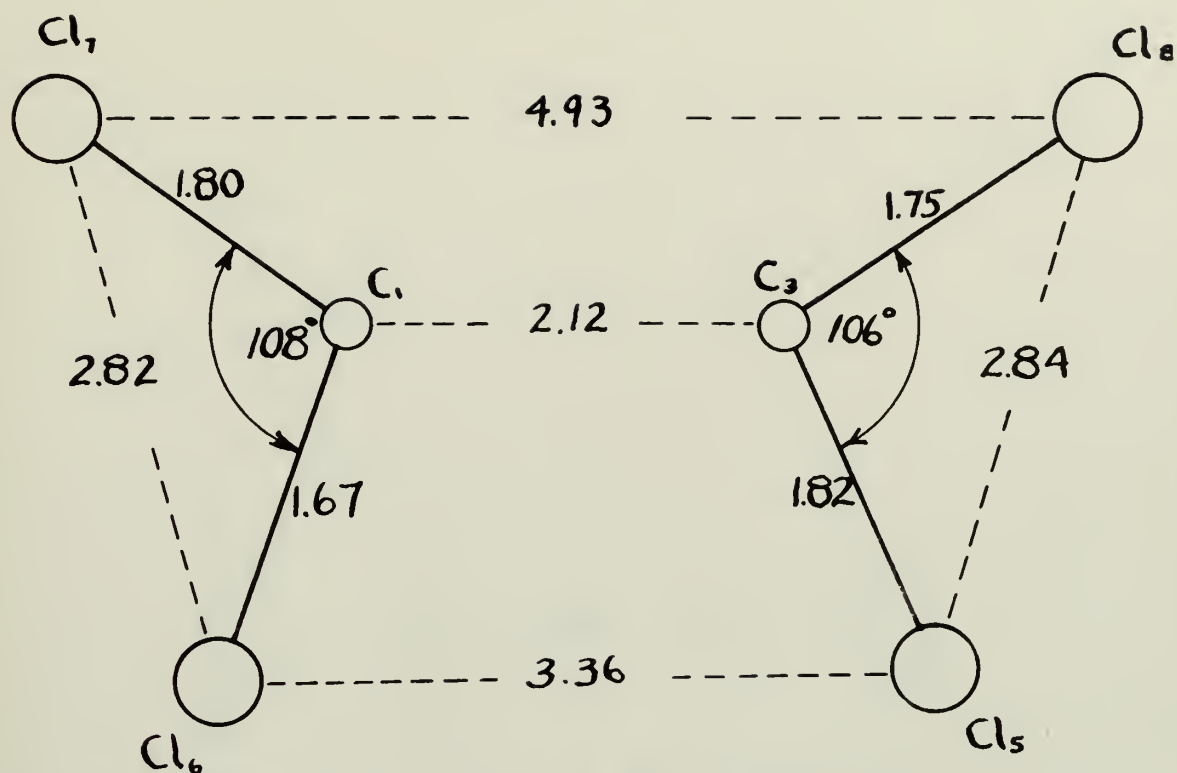


Figure 9

SKETCH SHOWING SOME VAN DER WAAL SEPARATIONS





DISTANCES IN PLANE $Y = \frac{1}{4}$

Figure 10

the carbon ring it can be seen that the chlorines have moved so as to equalize Cl - Cl interactions at the expense of deformation of the carbon ring. It is felt that the small amount of energy required for distortion of the ring is more than regained by equalization of the chlorine distances.

The optical behavior of the compound is of interest because the crystals show extinction parallel to the needle axis which the study has shown not to be the unique axis. In the monoclinic case, the orientation of the indicatrix must conform to the crystal symmetry and one axis thereof must coincide with the b axis of the unit cell. Ordinarily this is the only restriction on indicatrix orientation except that its other two axis must obviously lie in the ac plane taking any position in this plane but of course remaining at right angles to each other. For C_4Cl_8 the conclusion is that one of the two indicatrix axes in the ac plane lies parallel to c. This might be expected since the strings of molecules also lie parallel to c as does the fourfold alternating axis of the idealized molecule. The remaining indicatrix axis must then lie normal to c. It is believed that this optical behavior is good evidence in support of the conclusion that the molecular symmetry approximates closely to $\bar{4}m$.

The common ring is can be seen that the distances have moved on as the angles α - β increase at the expense of deformation of the carbon ring. It is said that the small amount of energy required for distortion of the ring is more than regained by equalization of the valence distances.

The optical behavior of the compound is of interest because the crystals show extinction parallel to the ac axis which the study has shown not to be the unique axis. In the monoclinic case, the extinction of the indicatrix must conform to the crystal symmetry and one axis necessarily must coincide with the b axis of the unit cell. Ordinarily this is the only restriction on indicatrix extinction except that the other two axes must necessarily lie in the ac plane taking any position in this plane but of course remaining at right angles to each other. But taking the conclusion is that one of the two indicatrices lies in the ac plane also parallel to b . This might be expected since the stretching of molecules also lie parallel to b as does the b axis of alternating axis of the identical molecules. The remaining indicatrix axis must then lie normal to b . It is believed that this optical behavior is good evidence in support of the conclusion that the molecular symmetry approximates closely to C_{2v} .

The puckering of the carbon ring is considerable, the dihedral angle being about 16° . From an examination of the literature this appears to be the first direct evidence of a non-planar cyclobutane ring. Edgell⁽¹⁰⁾ from the infra-red and Raman spectra study of C_4F_8 concludes that the ring is planar with a molecular symmetry D_{4h} . Preliminary results of electron diffraction studies of the same molecule by Livingston indicate that the ring is puckered. Spectroscopic studies of C_4H_8 are interpreted by Wilson⁽²⁰⁾ to show the molecular symmetry is not C_{2v} but rather D_{4h} . Dunitz' X-ray study of tetraphenyl cyclobutane shows the ring carbons to lie in a single plane, a symmetry center for the molecule being required for the space group.

Individual C-Cl distances are erratic because of poor carbon peaks in the Fourier sections. However they average out to 1.75 \AA , which is very close to the distance of 1.76 \AA observed by Pauling and Brockway⁽¹⁵⁾ in electron diffraction studies of CCl_4 . In liquid carbon tetrachloride Bray and Gingrich⁽³⁾ have observed the corresponding value as 1.74 \AA . For chlorines bonded to the same carbon atom an average separation of 2.82 \AA is found in C_4Cl_8 . A value of 2.86 \AA is reported by Pauling and Brockway as well as by Cosslett and de Laszlo⁽⁷⁾ in independent investigations of gaseous CCl_4 .

The presence of the carbon ring is essential.

The observed angle being about 10° , there is no doubt

of the literature this appears to be the first direct

evidence of a non-planar cyclobutane ring. (10)

From the infrared and Raman spectra study of C_4H_6 con-

cluded that the ring is planar with a molecular symmetry

D_{2h} . (11) Recently results of electron diffraction studies

of the same molecule by Leung and co-workers (12) and the ring

is planar. Spectroscopic studies of C_4H_6 and isomer-

ed by Wilson (13) as well as molecular symmetry is not

C_{2v} but rather D_{2h} . (14) X-ray study of tetramethyl-

ethylene shows the ring carbon to lie in a plane

plane, a symmetry center for the molecule being required

for the space group.

Dehydrohalogenation of alkyl halides and alkyl

halide bonds in the E2 reaction. However they

average out to 1.75 \AA . which is very close to the distance

of 1.75 \AA . observed by Pauling and Hildebrand (15) in elec-

tron diffraction studies of CH_4 . In liquid carbon

tetrachloride (16) and (17) have observed the

corresponding value as 1.75 \AA . for chlorine bonded to

the same carbon atom an average separation of 2.57 \AA .

is found in CH_4 . A value of 2.57 \AA . is reported by

Pauling and Hildebrand as well as by Connerly and co-workers (18)

in independent investigations of gaseous CH_4 .

Eisenstein⁽¹¹⁾ found the separation to be 2.95 \AA. at 27°C from X-ray studies for the liquid. The Cl-C-Cl angles observed in C_4Cl_8 were all slightly less than tetrahedral.

Carbon-Carbon bond lengths are not too accurate but the average value is indicative of a departure from the "normal" value of 1.54 \AA. The following table summarizes C-C spacings in compounds containing cyclobutane rings. In every case the values are greater than the normal value.

<u>Investigator</u>	<u>Compound</u>	<u>C-C</u> (\AA.)
Dunitz	Tetraphenyl- cyclobutane	1.585 ± 0.02 1.555 ± 0.02 } Avg. 1.57
Bauer & Beach ⁽¹⁾	Methylene (17) cyclobutane	1.56 ± 0.03
Shand, Schomaker, & Fischer	Methylene cyclobutane	1.55 ± 0.02
Lipscomb and Schomaker ⁽¹³⁾	Dimethyl ketene dimer	1.56 ± 0.05
Livingston	Perfluoro- cyclobutane (C_4F_8)	1.60
This investigation	C_4Cl_8	1.59 1.55 } Avg. 1.57

Preliminary X-ray analysis of dinaphthylene cyclobutane by Dunitz and Weissman⁽⁹⁾ indicate that C-C distances in the central ring may be longer than 1.54 \AA. also. They report that the molecule has a center of symmetry which means the ring must be planar.

The average C-C-C angle of 86.5° is of course only indicative of the puckering of the ring and cannot be taken as a final value since more accurate carbon positions are yet to be obtained.

SUGGESTIONS FOR FURTHER STUDY

In any refinement procedure one may employ, the atomic coordinates of the chlorine atoms will change little if at all. There does remain the problem of tiling down the positions of the carbon atoms. There are methods that may be used to improve the structure determination.

It has been mentioned previously that many relatively intense reflections were observed at high values of $(\sin \theta)/\lambda$. This indicates that probably there are numerous amplitudes of considerable magnitude beyond the maximum angle observable with Cu $K\alpha$ radiation but which still would contribute substantially to the Fourier summation. The incomplete series gives rise to a rippling effect which results in a displacement of maxima, particularly those of carbon atoms, from their true positions. It is desirable to obtain additional terms in the series to smooth out these ripples. Photographs taken with $M\alpha$ $K\alpha$ radiation should serve to pick up reflections further out in the reciprocal lattice. Incorporation of those additional amplitudes in the Fourier series should then lead to more accurate positions for carbon atoms.

There is a less desirable procedure that may be

In any refinement procedure one may suppose the
 would maintain the relative areas will change
 little if at all. There are some cases where the
 they show the position of the peaks. There
 the peaks that may be used to locate the
 position.

It has been mentioned previously that very relatively
 intense reflections were observed at high values of
 (sin θ)/ λ . This indicates that possibly there are
 numerous reflections of considerable intensity beyond the
 maximum angle observed with the radiation but which
 still would contribute substantially to the Fourier
 summation. The incomplete series gives rise to a ringing
 effect which results in a displacement of maxima, pos-
 sibly from the center of the peak, from their true posi-
 tion. It is desirable to obtain additional data in
 the series to correct for these effects. Photographs
 taken with a λ radiation should serve to pick up the
 positions further out in the reciprocal lattice. Inter-
 position of these additional amplitudes in the Fourier
 series should lead to more accurate positions for
 lattice planes.

There is a less desirable procedure that may be

followed but which is considered adequate by many in the field. The parameter values given by the Fourier synthesis of observed amplitudes are used to calculate structure amplitudes for the observed range of $(\sin \theta)/\lambda$. These calculated amplitudes are put through a Fourier synthesis which, since this series also is somewhat incomplete, will not reproduce exactly the peak positions used to obtain the calculated Fourier coefficients. The resulting small shift in position of each peak is applied with reversed sign as a correction to the corresponding atomic positions as given by the experimental Fourier synthesis.

Since carbon maxima may be displaced and ill-defined in the presence of the high chlorine peaks, it would be desirable if the Fourier syntheses could be calculated in such a way that the contributions of the chlorines to the series would not be included. Such a procedure was partially successful in the structure determination of UF_6 in the sense that when uranium peaks were subtracted out, rather well defined peaks for the light fluorine atoms remained. The method of attack was first to determine a scattering factor curve for uranium. Then structure factors were calculated for the U atoms alone and subtracted from the observed values. This left a residue which was taken as the contribution from fluorine atoms.

calculated and which is considered adequate by many in the field. The parameter values given by the Fourier synthesis of observed amplitudes are used to calculate structure amplitudes for the observed range of h and k . These calculated amplitudes are put through a Fourier synthesis which, above this range, also is somewhat incomplete, will not reproduce exactly the peak positions used to obtain the calculated Fourier coefficients. The resulting small shift in position of each peak is applied with reversed sign as a correction to the corresponding atomic positions as given by the experimental Fourier synthesis.

Since known metals may be disordered and ill-defined in the presence of the high electron beam, it would be desirable if the Fourier synthesis could be calculated in such a way that the contributions of the electrons to the series would not be limited. Such a procedure was partially successful in the structure determination of U_3O_8 in the sense that when certain peaks were subtracted out, better well defined peaks for the light fluorine atoms remained. The series of U_3O_8 was first to determine a scattering factor curve for uranium. Then atomic factor were calculated for the U atoms alone and subtracted from the observed values. This left a residual which was taken as the contribution from fluorine atoms.

Fourier calculations with the residue gave light atom peaks and enabled the investigators to obtain approximate atomic coordinates. This same procedure could probably be carried out for C_4Cl_8 but the determination of the experimental form factor for chlorine is at best a rather uncertain procedure.

positive relationship with the results gave little room
 for the results to indicate the importance of certain aspects
 of the results. This same procedure should
 probably be carried out for the other two experiments
 of the experimental design. The results of the first
 a rather complete analysis.

PART II

FURTHER STUDY OF THE STRUCTURE OF C_8F_{12}

[illegible]

INTRODUCTION

The first structure work on the dimer of hexafluorobutadiene, C_8F_{12} , was done by Dr. R. W. Broge⁽²¹⁾ in this Laboratory. The trial model employed was based on a "chair" configuration of the three cyclobutane rings fused at 120° angles to one another. Reasons for the choice of such a model are reviewed in his work. He found the unit cell to be triclinic and to simplify the problem based his analysis on a face-centered triclinic unit of $\underline{a_1}' = 9.95 \text{ \AA.}$ $\alpha' = 86.2^\circ$

$$\underline{a_2}' = 7.39 \text{ \AA.} \quad \beta' = 84.8^\circ$$

$$\underline{a_3}' = 13.20 \text{ \AA.} \quad \gamma' = 86.8^\circ$$

containing one molecule per lattice point. Since no positive pyroelectric effect was observed the molecule was believed to have a center of symmetry. Using zero-layer a' - axis data with the centrosymmetric model he determined a set of atomic parameters which, however, led to erratic C-C and C-F bond lengths and to poor agreement between calculated and observed amplitudes. It was clear that the structure problem required further study.

Since for triclinic lattices the choice of a

The first structure work on the alkyl of base-
 fluorosulfonates, $\text{C}_2\text{F}_5\text{SO}_3\text{H}$, was done by Dr. E. N. Blythe
 in this laboratory. The vital model synthesis was based
 on a 'chain' configuration of the three substituents
 rings fused at 120° angles to one another, persons
 for the choice of such a model are reviewed in his work.
 He found the model call to be realistic and as slightly
 the problem based his analysis on a face-centered cubi-

$$\begin{aligned} \frac{a_1}{a_2} &= 0.95 \text{ \AA.} & \lambda' &= 0.95^\circ \\ \frac{a_2}{a_3} &= 1.25 \text{ \AA.} & \delta' &= 94.5^\circ \\ \frac{a_3}{a_4} &= 1.35 \text{ \AA.} & \gamma' &= 98.5^\circ \end{aligned}$$

containing one molecule per lattice point. Since no
 positive pyroelectric effect was observed the molecule
 was believed to have a center of symmetry. Using info-
 layer α' - data only with the centrosymmetric model he
 determined a set of atomic parameters which, however,
 led to electric C-S and C-F bond lengths and to poor
 agreement between calculated and observed amplitudes.
 It was clear that the structure problem required further
 study.

Since the previous studies the choice of a

structural unit is not indicated by symmetry, Buerger has recommended that such lattices be reported in terms of what he calls the "reduced primitive cell." This is a unit the edges of which have the three shortest translations in the lattice and the axes of which are, labelled such that $\underline{a}_1 < \underline{a}_2 < \underline{a}_3$. An additional requirement is that the interaxial angles α , β , and γ are all obtuse. It was thought that if all reflections that might be observed were indexed on the basis of this unit the problem might be clarified and some progress might be made toward the final solution.

Figure 12 shows the face centered unit used by Broge together with the primitive reduced cell employed in the present study. It is seen that $\underline{a}_1 = \underline{BD}$, $\underline{a}_2 = \underline{DE}$, and $\underline{a}_3 = \underline{AB}$. The transformation from the compound to the primitive unit is:

$$\underline{a}_1 = \frac{-\underline{a}_2' + \underline{a}_1'}{2}$$

$$\underline{a}_2 = \frac{-\underline{a}_1' - \underline{a}_2'}{2}$$

$$\underline{a}_3 = \frac{-\underline{a}_3' + \underline{a}_2'}{2}$$

structural unit is not indicated by symmetry. However, her recommendations that such lattices be treated in terms of what he calls the "reduced primitive cell." This is a unit the edges of which have the same direction as the edges of the lattice and the area of which is equal to that of the lattice. An additional negative result is that the interaxial angles α, β, γ are all obtained. It was thought that if all reflections that might be observed were indexed on the basis of this unit the problem might be simplified and some progress might be made toward the final solution.

Figure 12 shows the face centered unit used by Bragg together with the primitive reduced cell employed in the present study. It is seen that $a_1 = a_2 = a_3 = a$ and $\alpha_1 = \alpha_2 = \alpha_3 = 120^\circ$. The transformation from the compound to the primitive unit is:

$$\frac{a_1}{2} = \frac{a_2}{2} = \frac{a_3}{2} = \frac{a}{2}$$

$$\frac{\alpha_1}{2} = \frac{\alpha_2}{2} = \frac{\alpha_3}{2} = \frac{\alpha}{2}$$

$$\frac{a_1}{2} = \frac{a_2}{2} = \frac{a_3}{2} = \frac{a}{2}$$

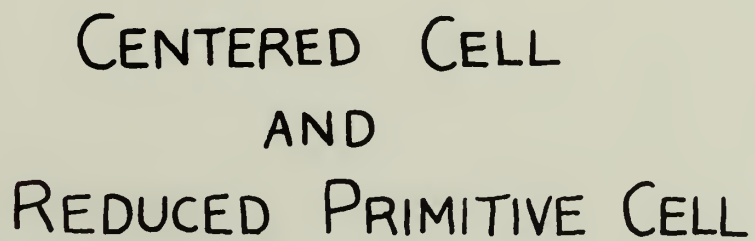


Figure 12

The present work was based on the centrosymmetric model. Although practically complete data for the primitive cell were obtained, no new atomic coordinates have been assigned and the structure still awaits solution. It is to be understood that the work reported herein was done prior to the investigation of the structure of octochlorocyclobutane. In view of the fact that the carbon ring is puckered in C_4Cl_8 , it may be that the rings in C_8F_{12} are not planar. If this be true a new trial model having no center of symmetry must be considered.

The present work was based on the centrosymmetric

model. Although practically complete data for the primitive cell were obtained, no new atomic coordinates have been assigned and the structure still awaits solution. It is to be understood that the work reported

herein was done prior to the investigation of the structure of $\text{CaSO}_4 \cdot \frac{1}{2}\text{H}_2\text{O}$. In view of the fact that the carbon atom is positioned in CaSO_4 , it may be that the atoms in CaSO_4 are not planar. If this be true a new trial model having no center of symmetry must be considered.

EXPERIMENTAL PROCEDURE

Single crystals of the compound were grown under vacuum by sublimation in thin-walled glass capillaries. The procedure is described by Broge and is a standard procedure in this Laboratory for crystals having high vapor pressures. In this study the capillaries were about 1 mm. in diameter and wall thickness averaged 0.01 mm. as measured under a microscope fitted with a micrometer eyepiece.

The crystals were mounted on the goniometer head such that the face of growth in the capillary was perpendicular to the rotation axis. Oscillation photographs were used to locate rational directions and to align the crystals for Weissenberg photography. Since the various repeat distances for rational directions could be calculated from Broge's work it was a simple matter to identify these directions on the photographs. Four crystals were photographed and the rational directions found may be described as follows:

<u>Crystal number</u>	<u>Repeat distance ($\text{\AA}.$)</u>	<u>Description</u>
1	6.3	$\underline{a_2}$ of reduced unit
2	6.0	$\underline{a_1}$ of reduced unit
3	6.3	$\underline{a_2}$ of reduced unit
4	7.4	$\underline{a_2}$ of centered cell.

The single crystals of the polymer were grown under vacuum by annealing in thin-walled glass capillaries. The procedure is described by Stoye and his students in this laboratory for systems having high vapor pressures. In this study the capillaries were about 1 mm. in diameter and well shrouded except for a 0.01 mm. diameter central microscope filament with a miniature syringe. The crystals were mounted on the condenser head such that the face of growth in the capillary was perpendicular to the rotation axis. Oscillation photographs were used to locate rotational directions and to align the crystals for x-ray diffraction photography. Since the various repeat distances for rotational directions could be calculated from Stoye's work it was a simple matter to identify these directions on the photographs. Four crystals were photographed and the rotational directions found may be described as follows:

Crystal number	Repeat distance (Å.)	Orientation
1	6.3	$\frac{1}{2}$ of reduced unit
2	6.0	$\frac{1}{2}$ of reduced unit
3	6.3	$\frac{1}{2}$ of reduced unit
4	7.4	$\frac{1}{2}$ of reduced unit

Crystal #1 was cracked and gave separation of spots; it was discarded after #3 was obtained.

Complete zero and higher layer equi-inclination Weissenberg photographs of all samples were taken with Cu K α radiation using the triple-film technique. The films were given exposure times of thirty minutes and four hours for each layer in order to be able to read spots over a wide range of intensity. Zero-layer NaCl reflections were superimposed on separate zero-layer photographs of C₈F₁₂ for good lattice constant measurement.

Indexing the Reflections.

The problem was simplified in that the reciprocal lattice of the primitive cell was known. In that lattice it was thus possible to calculate distances and angles which served to identify unequivocally the reflections on the films. Reflections from crystals 1, 2, and 3 were easily indexed. For crystal #4 it was necessary to choose an appropriate reciprocal lattice and the corresponding direct cell for use in indexing reflections and then transform indices so that they would refer to the reduced unit. The cell chosen was:

$$\begin{array}{ll} \underline{a_1}'' = 6.03 \text{ \AA} & \alpha'' = 57^\circ \\ \underline{a_2}'' = 7.39 & \beta'' = 74^\circ \\ \underline{a_3}'' = 7.76 & \gamma'' = 55.5^\circ \end{array}$$

Circuit A1 was checked and gave separation of spots.
It was discarded after it was obtained.

Complete sets and higher order reflections
were photographed at all angles with
Cu K α radiation using the typical technique. The
films were given exposure times of thirty minutes and
four hours for each layer in order to be able to scan
spots over a wide range of intensity. Two-layer and
reflections were photographed as separate sets.
Photographs of high order reflections were
obtained.

Indexing the reflections.

The problem was simplified in that the reciprocal
lattice of the primitive cell was known. In that lattice
it was thus possible to calculate distances and angles
which served to identify unambiguously the reflections
on the films. Reflections from crystals 1, 2, and 3
were easily indexed. For crystal 4 it was necessary
to choose an appropriate reciprocal lattice and the corresponding direct cell for use in indexing reflections and
then translate indices so that they would refer to the
reduced unit. The cell chosen was:

$$\begin{aligned} \underline{a}_1'' &= 6.01 \text{ \AA} \\ \underline{a}_2'' &= 7.25 \\ \underline{a}_3'' &= 7.75 \end{aligned}$$

The transformation to the primitive cell is:

$$\underline{a}_1 = \underline{a}_1''$$

$$\underline{a}_2 = \underline{a}_2'' - \underline{a}_1''$$

$$\underline{a}_3 = \underline{a}_3'' - \underline{a}_2'' .$$

Determination of the Lattice constants.

Using the cell constants determined by Broge for the centered unit the reciprocal lattice for the reduced cell has

$$\underline{a}_1^* = 0.1891 \text{ \AA}^{-1} \quad \alpha^* = 70.8^\circ$$

$$\underline{a}_2^* = 0.1742 \quad \beta^* = 66.3^\circ$$

$$\underline{a}_3^* = 0.1525 \quad \gamma^* = 68.0^\circ$$

However measurements on zero-layer Weissenberg photographs taken in the present study lead to

$$\underline{a}_1^* = 0.1890 \pm 0.0002 \text{ \AA}^{-1} \quad \alpha^* = 69.3^\circ$$

$$\underline{a}_2^* = 0.1772 \pm 0.0002 \quad \beta^* = 66.3^\circ$$

$$\underline{a}_3^* = 0.1545 \pm 0.0002$$

The spacing of \underline{a}_2 was measured from an oscillation photograph upon which NaCl reflections had been superimposed and was found to be 6.29 \AA . Using this value with appropriate formulae the reciprocal lattice angle γ^*

The transmission to the primary cell is

$$\frac{I_1}{I_0} = \frac{1}{1 + \frac{1}{Q^2}}$$

$$\frac{I_2}{I_0} = \frac{1}{1 + \frac{1}{Q^2}}$$

$$\frac{I_3}{I_0} = \frac{1}{1 + \frac{1}{Q^2}}$$

Determination of the lattice constants.

Using the cell constants determined by X-ray the scattering angle the reciprocal lattice for the reduced

cell has

$$\frac{a_1^*}{a_1} = 0.1001 \pm 0.0002 \quad \alpha = 70.8^\circ$$

$$\frac{a_2^*}{a_2} = 0.1143 \quad \beta = 64.3^\circ$$

$$\frac{a_3^*}{a_3} = 0.1125 \quad \gamma = 68.0^\circ$$

However measurements on zero-layer reflexions photographs taken in the present study lead to

$$\frac{a_1^*}{a_1} = 0.1002 \pm 0.0002 \quad \alpha = 69.3^\circ$$

$$\frac{a_2^*}{a_2} = 0.1172 \pm 0.0002 \quad \beta = 66.3^\circ$$

$$\frac{a_3^*}{a_3} = 0.1045 \pm 0.0002$$

The spacing of a_3^* was measured from an oscillation photo-

graph upon which well reflections had been superimposed

and was found to be 0.10 ± 0.001 . Using this value with

appropriate formulae the reciprocal lattice angle γ^*

was determined to be 67.4° . Direct cell constants are then

$$\underline{a_1} = 6.02 \text{ \AA} \quad \alpha = 103.6^\circ$$

$$\underline{a_2} = 6.29 \quad \beta = 107.9^\circ$$

$$\underline{a_3} = 7.27 \quad \gamma = 106.4^\circ$$

for the primitive reduced unit. These values lead to a unit cell volume of 235.2 \AA^3 and an X-ray density of 2.29 gm./cc. Broge lists 240.7 \AA^3 and 2.23 gm./cc. as a result of his study. It is to be noted that he had to employ the method of angular lag to determine angles in reciprocal space.

Intensity Measurement.

The relative intensities were determined by visual comparison of the reflections with the intensity scale described in Part I. Values of $(\sin \theta)/\lambda$ were computed graphically rather than from film measurements. The Lorentz and Polarization and the Tunell factor where applicable were applied to the intensities to obtain relative F^2 values. By careful cross-calibration all data were reduced to the four hour zero layer a_1 axis photograph. Excellent checks were obtained for reflections common to two or more films. The relative F^2 values are listed in Table III.

TABLE III

Rel.			Rel.		
hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$	hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$
010	0.089	950	111	0.201	280
020	0.178	800	121	0.272	1.8
030	0.255	660	131	0.357	1750
040	0.355	24	141	0.435	13
050	0.443	176	151	0.526	0
060	0.533	2.4	161	0.610	-
070	0.620	0	10 $\bar{1}$	0.084	1300
100	0.084	1600	11 $\bar{1}$	0.136	150
110	0.156	370	12 $\bar{1}$	0.208	5800
120	0.234	40	13 $\bar{1}$	0.292	52
130	0.311	72	14 $\bar{1}$	0.376	110
140	0.402	100	15 $\bar{1}$	0.467	111
150	0.486	33	16 $\bar{1}$	0.551	0
160	0.578	-	17 $\bar{1}$	0.636	0
1 $\bar{1}$ 0	0.097	2000	1 $\bar{1}$ 1	0.123	85
1 $\bar{2}$ 0	0.162	100	1 $\bar{2}$ 1	0.188	94
1 $\bar{3}$ 0	0.240	1000	1 $\bar{3}$ 1	0.272	630
1 $\bar{4}$ 0	0.331	1750	1 $\bar{4}$ 1	0.357	5
1 $\bar{5}$ 0	0.415	3.6	1 $\bar{5}$ 1	0.441	159
1 $\bar{6}$ 0	0.565	35	1 $\bar{6}$ 1	0.532	110
1 $\bar{7}$ 0	0.636	1.2	1 $\bar{1}$ $\bar{1}$	0.130	62
001	0.077	660	1 $\bar{2}$ $\bar{1}$	0.149	980
011	0.136	625	1 $\bar{3}$ $\bar{1}$	0.234	610
021	0.218	140	1 $\bar{4}$ $\bar{1}$	0.318	230
031	0.300	145	1 $\bar{5}$ $\bar{1}$	0.396	410
041	0.388	14	1 $\bar{6}$ $\bar{1}$	0.480	195
051	0.475	12	1 $\bar{7}$ $\bar{1}$	0.571	3
061	0.564	2	002	0.154	337
01 $\bar{1}$	0.094	2300	012	0.204	5595
02 $\bar{1}$	0.166	350	022	0.274	580
03 $\bar{1}$	0.248	60	032	0.351	22
04 $\bar{1}$	0.334	16	042	0.434	64
05 $\bar{1}$	0.422	62	052	0.518	37
06 $\bar{1}$	0.511	2.7	062	0.604	6
07 $\bar{1}$	0.597	6.7	01 $\bar{2}$	0.147	155
101	0.143	860	02 $\bar{2}$	0.189	900

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[illegible]

TABLE III (Continued)

Rel.			Rel.		
hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$	hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$
03 $\bar{2}$	0.254	15	043	0.485	37
04 $\bar{2}$	0.332	613	053	0.565	0
05 $\bar{2}$	0.414	14.7	063	0.645	0
06 $\bar{2}$	0.495	39			
07 $\bar{2}$	0.584	22	01 $\bar{3}$	0.214	370
			02 $\bar{3}$	0.235	8
102	0.208	430	03 $\bar{3}$	0.282	19
112	0.259	1000	04 $\bar{3}$	0.347	340
122	0.331	6	05 $\bar{3}$	0.421	96
132	0.402	2	06 $\bar{3}$	0.498	40
142	0.486	47	07 $\bar{3}$	0.580	0
152	0.571	0			
			103	0.379	22
10 $\bar{2}$	0.149	330	113	0.321	25
11 $\bar{2}$	0.162	7.5	123	0.389	10
12 $\bar{2}$	0.214	5	133	0.461	52
13 $\bar{2}$	0.285	600	143	0.538	75
14 $\bar{2}$	0.370	270	153	0.545	0
15 $\bar{2}$	0.454	0			
16 $\bar{2}$	0.538	-	10 $\bar{3}$	0.214	108
17 $\bar{2}$	0.623	-	11 $\bar{3}$	0.214	6970
			12 $\bar{3}$	0.246	53
112	0.175	190	13 $\bar{3}$	0.305	360
122	0.240	57	14 $\bar{3}$	0.376	370
132	0.318	19	15 $\bar{3}$	0.454	26
142	0.396	85	16 $\bar{3}$	0.538	-
152	0.480	218	17 $\bar{3}$	0.590	-
162	0.565	37			
			113	0.246	210
11 $\bar{2}$	0.188	510	123	0.305	70
12 $\bar{2}$	0.208	900	133	0.370	50
13 $\bar{2}$	0.252	2200	143	0.447	80
14 $\bar{2}$	0.324	2.9	153	0.532	13
15 $\bar{2}$	0.396	17	163	0.610	15
16 $\bar{2}$	0.473	112			
17 $\bar{2}$	0.519	6.4	11 $\bar{3}$	0.253	960
			12 $\bar{3}$	0.260	1100
003	0.230	590	13 $\bar{3}$	0.292	180
013	0.275	760	14 $\bar{3}$	0.344	180
023	0.338	72	15 $\bar{3}$	0.409	285
033	0.407	10.8	16 $\bar{3}$	0.480	16

TABLE III (Continued)

Wavelength (microns)	Refractive Index	Dispersion	Wavelength (microns)	Refractive Index	Dispersion
0.35	0.400	0.000	0.35	0.400	0.000
0.40	0.395	0.000	0.40	0.395	0.000
0.45	0.390	0.000	0.45	0.390	0.000
0.50	0.385	0.000	0.50	0.385	0.000
0.55	0.380	0.000	0.55	0.380	0.000
0.60	0.375	0.000	0.60	0.375	0.000
0.65	0.370	0.000	0.65	0.370	0.000
0.70	0.365	0.000	0.70	0.365	0.000
0.75	0.360	0.000	0.75	0.360	0.000
0.80	0.355	0.000	0.80	0.355	0.000
0.85	0.350	0.000	0.85	0.350	0.000
0.90	0.345	0.000	0.90	0.345	0.000
0.95	0.340	0.000	0.95	0.340	0.000
1.00	0.335	0.000	1.00	0.335	0.000
1.05	0.330	0.000	1.05	0.330	0.000
1.10	0.325	0.000	1.10	0.325	0.000
1.15	0.320	0.000	1.15	0.320	0.000
1.20	0.315	0.000	1.20	0.315	0.000
1.25	0.310	0.000	1.25	0.310	0.000
1.30	0.305	0.000	1.30	0.305	0.000
1.35	0.300	0.000	1.35	0.300	0.000
1.40	0.295	0.000	1.40	0.295	0.000
1.45	0.290	0.000	1.45	0.290	0.000
1.50	0.285	0.000	1.50	0.285	0.000
1.55	0.280	0.000	1.55	0.280	0.000
1.60	0.275	0.000	1.60	0.275	0.000
1.65	0.270	0.000	1.65	0.270	0.000
1.70	0.265	0.000	1.70	0.265	0.000
1.75	0.260	0.000	1.75	0.260	0.000
1.80	0.255	0.000	1.80	0.255	0.000
1.85	0.250	0.000	1.85	0.250	0.000
1.90	0.245	0.000	1.90	0.245	0.000
1.95	0.240	0.000	1.95	0.240	0.000
2.00	0.235	0.000	2.00	0.235	0.000
2.05	0.230	0.000	2.05	0.230	0.000
2.10	0.225	0.000	2.10	0.225	0.000
2.15	0.220	0.000	2.15	0.220	0.000
2.20	0.215	0.000	2.20	0.215	0.000
2.25	0.210	0.000	2.25	0.210	0.000
2.30	0.205	0.000	2.30	0.205	0.000
2.35	0.200	0.000	2.35	0.200	0.000
2.40	0.195	0.000	2.40	0.195	0.000
2.45	0.190	0.000	2.45	0.190	0.000
2.50	0.185	0.000	2.50	0.185	0.000
2.55	0.180	0.000	2.55	0.180	0.000
2.60	0.175	0.000	2.60	0.175	0.000
2.65	0.170	0.000	2.65	0.170	0.000
2.70	0.165	0.000	2.70	0.165	0.000
2.75	0.160	0.000	2.75	0.160	0.000
2.80	0.155	0.000	2.80	0.155	0.000
2.85	0.150	0.000	2.85	0.150	0.000
2.90	0.145	0.000	2.90	0.145	0.000
2.95	0.140	0.000	2.95	0.140	0.000
3.00	0.135	0.000	3.00	0.135	0.000
3.05	0.130	0.000	3.05	0.130	0.000
3.10	0.125	0.000	3.10	0.125	0.000
3.15	0.120	0.000	3.15	0.120	0.000
3.20	0.115	0.000	3.20	0.115	0.000
3.25	0.110	0.000	3.25	0.110	0.000
3.30	0.105	0.000	3.30	0.105	0.000
3.35	0.100	0.000	3.35	0.100	0.000
3.40	0.095	0.000	3.40	0.095	0.000
3.45	0.090	0.000	3.45	0.090	0.000
3.50	0.085	0.000	3.50	0.085	0.000
3.55	0.080	0.000	3.55	0.080	0.000
3.60	0.075	0.000	3.60	0.075	0.000
3.65	0.070	0.000	3.65	0.070	0.000
3.70	0.065	0.000	3.70	0.065	0.000
3.75	0.060	0.000	3.75	0.060	0.000
3.80	0.055	0.000	3.80	0.055	0.000
3.85	0.050	0.000	3.85	0.050	0.000
3.90	0.045	0.000	3.90	0.045	0.000
3.95	0.040	0.000	3.95	0.040	0.000
4.00	0.035	0.000	4.00	0.035	0.000

TABLE III (Continued)

Rel.			Rel.		
hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$	hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$
I73	0.558	2.5	I44	0.383	120
004	0.307	25	I54	0.435	640
014	0.350	24	I64	0.499	16
024	0.405	620	I74	0.571	0
034	0.472	0	005	0.384	5.4
044	0.540	0	015	0.423	0
054	0.622	0	025	0.477	0
014	0.287	610	035	0.533	6.4
024	0.296	48	045	0.607	0
034	0.327	800	015	0.363	86
044	0.377	430	025	0.361	0
054	0.441	43	035	0.381	67
064	0.513	175	045	0.420	110
074	0.587	0	055	0.473	6
104	0.357	8	065	0.535	0
114	0.402	15	075	0.604	14.5
124	0.461	7	105	0.428	139
134	0.532	0	115	0.474	24
144	0.596	5	125	0.499	5
104	0.285	240	135	0.590	10
114	0.279	24	105	0.357	2300
124	0.298	900	115	0.344	2.2
134	0.337	415	125	0.331	200
144	0.396	18	135	0.382	370
154	0.461	88	145	0.428	4.6
164	0.538	-	155	0.486	0
174	0.616	-	165	0.558	-
I14	0.318	3	175	0.629	-
I24	0.369	21	I15	0.389	3.5
I34	0.434	63	I25	0.441	33
I44	0.506	0	I35	0.499	6
I54	0.584	0	I45	0.571	19
I14	0.331	73	I55	0.636	6.4
I24	0.324	1200	I15	0.402	185
I34	0.344	10	I25	0.389	8

TABLE III (Continued)

Left			Right		
λ	$\frac{S}{\lambda}$	λ	λ	$\frac{S}{\lambda}$	λ
1.00	0.000	1.00	1.00	0.000	1.00
1.01	0.000	1.01	1.01	0.000	1.01
1.02	0.000	1.02	1.02	0.000	1.02
1.03	0.000	1.03	1.03	0.000	1.03
1.04	0.000	1.04	1.04	0.000	1.04
1.05	0.000	1.05	1.05	0.000	1.05
1.06	0.000	1.06	1.06	0.000	1.06
1.07	0.000	1.07	1.07	0.000	1.07
1.08	0.000	1.08	1.08	0.000	1.08
1.09	0.000	1.09	1.09	0.000	1.09
1.10	0.000	1.10	1.10	0.000	1.10
1.11	0.000	1.11	1.11	0.000	1.11
1.12	0.000	1.12	1.12	0.000	1.12
1.13	0.000	1.13	1.13	0.000	1.13
1.14	0.000	1.14	1.14	0.000	1.14
1.15	0.000	1.15	1.15	0.000	1.15
1.16	0.000	1.16	1.16	0.000	1.16
1.17	0.000	1.17	1.17	0.000	1.17
1.18	0.000	1.18	1.18	0.000	1.18
1.19	0.000	1.19	1.19	0.000	1.19
1.20	0.000	1.20	1.20	0.000	1.20
1.21	0.000	1.21	1.21	0.000	1.21
1.22	0.000	1.22	1.22	0.000	1.22
1.23	0.000	1.23	1.23	0.000	1.23
1.24	0.000	1.24	1.24	0.000	1.24
1.25	0.000	1.25	1.25	0.000	1.25
1.26	0.000	1.26	1.26	0.000	1.26
1.27	0.000	1.27	1.27	0.000	1.27
1.28	0.000	1.28	1.28	0.000	1.28
1.29	0.000	1.29	1.29	0.000	1.29
1.30	0.000	1.30	1.30	0.000	1.30
1.31	0.000	1.31	1.31	0.000	1.31
1.32	0.000	1.32	1.32	0.000	1.32
1.33	0.000	1.33	1.33	0.000	1.33
1.34	0.000	1.34	1.34	0.000	1.34
1.35	0.000	1.35	1.35	0.000	1.35
1.36	0.000	1.36	1.36	0.000	1.36
1.37	0.000	1.37	1.37	0.000	1.37
1.38	0.000	1.38	1.38	0.000	1.38
1.39	0.000	1.39	1.39	0.000	1.39
1.40	0.000	1.40	1.40	0.000	1.40
1.41	0.000	1.41	1.41	0.000	1.41
1.42	0.000	1.42	1.42	0.000	1.42
1.43	0.000	1.43	1.43	0.000	1.43
1.44	0.000	1.44	1.44	0.000	1.44
1.45	0.000	1.45	1.45	0.000	1.45
1.46	0.000	1.46	1.46	0.000	1.46
1.47	0.000	1.47	1.47	0.000	1.47
1.48	0.000	1.48	1.48	0.000	1.48
1.49	0.000	1.49	1.49	0.000	1.49
1.50	0.000	1.50	1.50	0.000	1.50

TABLE III (Continued)

Rel.			Rel.		
hkl	$\frac{\sin \theta}{\lambda}$	$(F_{hkl})^2$	hkl	$\frac{\sin \theta}{\lambda}$	$(F_{hkl})^2$
I35	0.402	300	I66	0.571	0
I45	0.428	3.1	I76	0.623	0
I55	0.474	20	007	0.539	14
I65	0.526	3	017	0.570	11
I75	0.590	0	027	0.623	0
006	0.462	110	017	0.514	0
016	0.500	3	027	0.504	6
026	0.549	0	037	0.510	0
036	0.608	30	047	0.530	0
016	0.438	7.3	057	0.563	0
026	0.432	260	067	0.608	10.8
036	0.443	180	107	0.584	4
046	0.472	7.5	117	0.623	0
056	0.516	193	107	0.513	10
066	0.569	0	117	0.493	40
076	0.630	0	127	0.487	115
106	0.506	5	137	0.499	0
116	0.552	0	147	0.526	0
126	0.603	8.5	157	0.571	5.3
106	0.434	14	167	0.623	-
116	0.415	270	I17	0.545	105
126	0.422	40	I27	0.590	6
136	0.441	0	I37	0.643	1.1
146	0.474	80	I17	0.558	12
156	0.525	9	I27	0.538	110
166	0.590	-	I37	0.538	0
I16	0.467	125	I47	0.551	0
I26	0.519	4	I57	0.577	0
I36	0.571	1.6	I67	0.616	0
I46	0.640	3	008	0.616	0
I16	0.480	140	018	0.591	4
I26	0.467	18.5	028	0.578	0
I36	0.467	140	038	0.578	5.3
I46	0.486	180			
I56	0.519	0			

TABLE IV
(Continued)[illegible]

TABLE III (Continued)

Rel.			Rel.		
hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$	hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$
04 $\bar{8}$	0.592	50	201	0.227	400
05 $\bar{8}$	0.620	0	211	0.285	485
10 $\bar{3}$	0.597	14	221	0.350	42
11 $\bar{8}$	0.571	0	231	0.422	95
12 $\bar{8}$	0.564	1.6	241	0.499	17
13 $\bar{8}$	0.564	10.4	251	0.583	0
14 $\bar{8}$	0.584	0	20 $\bar{1}$	0.175	880
15 $\bar{8}$	0.622	0	21 $\bar{1}$	0.214	14
11 $\bar{8}$	0.624	4	22 $\bar{1}$	0.278	200
11 $\bar{3}$	0.629	6.1	23 $\bar{1}$	0.357	120
12 $\bar{8}$	0.616	0	24 $\bar{1}$	0.441	0
13 $\bar{8}$	0.603	2.6	25 $\bar{1}$	0.519	0
14 $\bar{8}$	0.616	0	26 $\bar{1}$	0.603	-
15 $\bar{8}$	0.636	0	211	0.169	314
02 $\bar{9}$	0.647	-	221	0.208	6550
03 $\bar{9}$	0.645	0	231	0.272	108
11 $\bar{9}$	0.640	14.7	241	0.350	17
12 $\bar{9}$	0.624	-	251	0.428	290
13 $\bar{9}$	0.624	-	261	0.512	1.7
14 $\bar{9}$	0.635	-	271	0.585	0
200	0.188	600	21 $\bar{1}$	0.208	4100
210	0.240	1180	22 $\bar{1}$	0.214	80
220	0.305	200	231	0.259	70
230	0.383	300	241	0.324	700
240	0.467	0	251	0.396	0
250	0.545	0	261	0.473	160
260	0.636	0	271	0.558	20
210	0.175	27.5	202	0.285	167
220	0.194	25.	212	0.337	13
230	0.259	500	222	0.402	71
240	0.324	130	232	0.473	52
250	0.402	15	242	0.551	17
260	0.487	120	252	0.629	0
270	0.571	1.8	20 $\bar{2}$	0.188	800
			21 $\bar{2}$	0.214	230
			22 $\bar{2}$	0.272	840

[illegible]

TABLE III (Continued)

Rel.			Rel.		
hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$	hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$
$\overline{2}3\overline{2}$	0.344	6	$\overline{2}53$	0.506	0
$\overline{2}4\overline{2}$	0.422	260	$\overline{2}63$	0.583	6.6
$\overline{2}5\overline{2}$	0.506	35	$\overline{2}1\overline{3}$	0.318	6.5
$\overline{2}6\overline{2}$	0.584	-	$\overline{2}2\overline{3}$	0.311	9
$\overline{2}12$	0.201	470	$\overline{2}3\overline{3}$	0.331	420
$\overline{2}22$	0.246	15	$\overline{2}4\overline{3}$	0.369	100
$\overline{2}32$	0.305	170	$\overline{2}5\overline{3}$	0.421	500
$\overline{2}42$	0.383	125	$\overline{2}6\overline{3}$	0.487	60
$\overline{2}52$	0.461	61	$\overline{2}7\overline{3}$	0.558	1.4
$\overline{2}62$	0.543	20	$\overline{2}8\overline{3}$	0.630	63
$\overline{2}72$	0.618	0	204	0.422	0
$\overline{2}1\overline{2}$	0.260	11	214	0.467	80
$\overline{2}2\overline{2}$	0.260	490	224	0.499	0
$\overline{2}3\overline{2}$	0.292	150	234	0.590	8.8
$\overline{2}4\overline{2}$	0.337	1.4	$20\overline{4}$	0.292	145
$\overline{2}5\overline{2}$	0.402	85	$21\overline{4}$	0.298	400
$\overline{2}6\overline{2}$	0.474	0	$22\overline{4}$	0.324	5.3
$\overline{2}7\overline{2}$	0.551	0	$23\overline{4}$	0.369	900
282	0.630	5.5	$24\overline{4}$	0.434	180
203	0.350	1500	$25\overline{4}$	0.506	0
213	0.402	16	$26\overline{4}$	0.577	26.6
223	0.461	80	$\overline{2}14$	0.311	90
233	0.532	5	$\overline{2}24$	0.357	1.4
243	0.603	13	$\overline{2}34$	0.415	10
$20\overline{3}$	0.235	200	$\overline{2}44$	0.486	70
$21\overline{3}$	0.246	74	$\overline{2}54$	0.558	15
$22\overline{3}$	0.292	300	$\overline{2}64$	0.630	5
$23\overline{3}$	0.344	13	$\overline{2}1\overline{4}$	0.389	110
$24\overline{3}$	0.422	1.9	$\overline{2}2\overline{4}$	0.376	2.3
$25\overline{3}$	0.499	177	$\overline{2}3\overline{4}$	0.389	190
$26\overline{3}$	0.577	0	$\overline{2}4\overline{4}$	0.415	2.8
$\overline{2}13$	0.253	1100	$\overline{2}5\overline{4}$	0.454	113
$\overline{2}23$	0.298	240	$\overline{2}6\overline{4}$	0.512	36
$\overline{2}33$	0.357	1900	$\overline{2}74$	0.572	21
$\overline{2}43$	0.428	34			

(Continued) THE STATE

1961	1962	1963	1964	1965	1966
0	000.0	000	0	000.0	000
1.1	000.0	000	000	000.0	000
2.2	000.0	000	000	000.0	000
3.3	000.0	000	000	000.0	000
4.4	000.0	000	000	000.0	000
5.5	000.0	000	000	000.0	000
6.6	000.0	000	000	000.0	000
7.7	000.0	000	000	000.0	000
8.8	000.0	000	000	000.0	000
9.9	000.0	000	000	000.0	000
10.0	000.0	000	000	000.0	000
11.1	000.0	000	000	000.0	000
12.2	000.0	000	000	000.0	000
13.3	000.0	000	000	000.0	000
14.4	000.0	000	000	000.0	000
15.5	000.0	000	000	000.0	000
16.6	000.0	000	000	000.0	000
17.7	000.0	000	000	000.0	000
18.8	000.0	000	000	000.0	000
19.9	000.0	000	000	000.0	000
20.0	000.0	000	000	000.0	000
21.1	000.0	000	000	000.0	000
22.2	000.0	000	000	000.0	000
23.3	000.0	000	000	000.0	000
24.4	000.0	000	000	000.0	000
25.5	000.0	000	000	000.0	000
26.6	000.0	000	000	000.0	000
27.7	000.0	000	000	000.0	000
28.8	000.0	000	000	000.0	000
29.9	000.0	000	000	000.0	000
30.0	000.0	000	000	000.0	000
31.1	000.0	000	000	000.0	000
32.2	000.0	000	000	000.0	000
33.3	000.0	000	000	000.0	000
34.4	000.0	000	000	000.0	000
35.5	000.0	000	000	000.0	000
36.6	000.0	000	000	000.0	000
37.7	000.0	000	000	000.0	000
38.8	000.0	000	000	000.0	000
39.9	000.0	000	000	000.0	000
40.0	000.0	000	000	000.0	000
41.1	000.0	000	000	000.0	000
42.2	000.0	000	000	000.0	000
43.3	000.0	000	000	000.0	000
44.4	000.0	000	000	000.0	000
45.5	000.0	000	000	000.0	000
46.6	000.0	000	000	000.0	000
47.7	000.0	000	000	000.0	000
48.8	000.0	000	000	000.0	000
49.9	000.0	000	000	000.0	000
50.0	000.0	000	000	000.0	000
51.1	000.0	000	000	000.0	000
52.2	000.0	000	000	000.0	000
53.3	000.0	000	000	000.0	000
54.4	000.0	000	000	000.0	000
55.5	000.0	000	000	000.0	000
56.6	000.0	000	000	000.0	000
57.7	000.0	000	000	000.0	000
58.8	000.0	000	000	000.0	000
59.9	000.0	000	000	000.0	000
60.0	000.0	000	000	000.0	000
61.1	000.0	000	000	000.0	000
62.2	000.0	000	000	000.0	000
63.3	000.0	000	000	000.0	000
64.4	000.0	000	000	000.0	000
65.5	000.0	000	000	000.0	000
66.6	000.0	000	000	000.0	000
67.7	000.0	000	000	000.0	000
68.8	000.0	000	000	000.0	000
69.9	000.0	000	000	000.0	000
70.0	000.0	000	000	000.0	000
71.1	000.0	000	000	000.0	000
72.2	000.0	000	000	000.0	000
73.3	000.0	000	000	000.0	000
74.4	000.0	000	000	000.0	000
75.5	000.0	000	000	000.0	000
76.6	000.0	000	000	000.0	000
77.7	000.0	000	000	000.0	000
78.8	000.0	000	000	000.0	000
79.9	000.0	000	000	000.0	000
80.0	000.0	000	000	000.0	000
81.1	000.0	000	000	000.0	000
82.2	000.0	000	000	000.0	000
83.3	000.0	000	000	000.0	000
84.4	000.0	000	000	000.0	000
85.5	000.0	000	000	000.0	000
86.6	000.0	000	000	000.0	000
87.7	000.0	000	000	000.0	000
88.8	000.0	000	000	000.0	000
89.9	000.0	000	000	000.0	000
90.0	000.0	000	000	000.0	000
91.1	000.0	000	000	000.0	000
92.2	000.0	000	000	000.0	000
93.3	000.0	000	000	000.0	000
94.4	000.0	000	000	000.0	000
95.5	000.0	000	000	000.0	000
96.6	000.0	000	000	000.0	000
97.7	000.0	000	000	000.0	000
98.8	000.0	000	000	000.0	000
99.9	000.0	000	000	000.0	000
100.0	000.0	000	000	000.0	000

TABLE III (Continued)

Rel.			Rel.		
hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$	hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$
205	0.493	27	$\bar{2}1\bar{6}$	0.545	16
215	0.538	51	$\bar{2}2\bar{6}$	0.512	94
225	0.596	2	$\bar{2}3\bar{6}$	0.506	9.2
			$\bar{2}4\bar{6}$	0.525	100
$20\bar{5}$	0.357	2.4	$\bar{2}5\bar{6}$	0.551	1.4
$21\bar{5}$	0.350	184	$\bar{2}6\bar{6}$	0.584	17
$22\bar{5}$	0.369	120	$\bar{2}7\bar{6}$	0.635	4.6
$23\bar{5}$	0.408	50			
$24\bar{5}$	0.461	630	207	0.635	0
$25\bar{5}$	0.519	0			
$26\bar{5}$	0.590	12.6	$20\bar{7}$	0.499	26
			$21\bar{7}$	0.486	68
$\bar{2}15$	0.383	18	$22\bar{7}$	0.486	40
$\bar{2}25$	0.428	115	$23\bar{7}$	0.506	245
$\bar{2}35$	0.480	74	$24\bar{7}$	0.533	0
$\bar{2}45$	0.545	100	$25\bar{7}$	0.583	6.4
$\bar{2}55$	0.616	3	$26\bar{7}$	0.636	-
$\bar{2}1\bar{5}$	0.461	0	$\bar{2}17$	0.525	14.6
$\bar{2}2\bar{5}$	0.447	150	$\bar{2}27$	0.564	0
$\bar{2}3\bar{5}$	0.447	72	$\bar{2}37$	0.617	0
$\bar{2}4\bar{5}$	0.467	118			
$\bar{2}5\bar{5}$	0.499	2.7	$\bar{2}1\bar{7}$	0.610	10
$\bar{2}6\bar{5}$	0.545	0	$\bar{2}2\bar{7}$	0.590	0
$\bar{2}7\bar{5}$	0.596	64	$\bar{2}3\bar{7}$	0.584	0
			$\bar{2}4\bar{7}$	0.584	12
206	0.564	7	$\bar{2}5\bar{7}$	0.603	0
216	0.609	2.9	$\bar{2}6\bar{7}$	0.636	12
$20\bar{6}$	0.428	29	$20\bar{8}$	0.571	0
$21\bar{6}$	0.415	0	$21\bar{8}$	0.558	47
$22\bar{6}$	0.428	450	$22\bar{8}$	0.558	0
$23\bar{6}$	0.454	53	$23\bar{8}$	0.571	1.8
$24\bar{6}$	0.499	9.1	$24\bar{8}$	0.590	9.0
$25\bar{6}$	0.551	8.4	$25\bar{8}$	0.629	7.6
$26\bar{6}$	0.610	-			
			$\bar{2}18$	0.617	25.6
$\bar{2}16$	0.454	8	$\bar{2}28$	0.636	0
$\bar{2}26$	0.493	0			
$\bar{2}36$	0.538	1.6	$20\bar{9}$	0.649	2.5
$\bar{2}46$	0.610	4	$21\bar{9}$	0.630	0

TABLE III (Continued)

Left			Right		
Year	Rate	Value	Year	Rate	Value
1950	0.000	0.000	1950	0.000	0.000
1951	0.000	0.000	1951	0.000	0.000
1952	0.000	0.000	1952	0.000	0.000
1953	0.000	0.000	1953	0.000	0.000
1954	0.000	0.000	1954	0.000	0.000
1955	0.000	0.000	1955	0.000	0.000
1956	0.000	0.000	1956	0.000	0.000
1957	0.000	0.000	1957	0.000	0.000
1958	0.000	0.000	1958	0.000	0.000
1959	0.000	0.000	1959	0.000	0.000
1960	0.000	0.000	1960	0.000	0.000
1961	0.000	0.000	1961	0.000	0.000
1962	0.000	0.000	1962	0.000	0.000
1963	0.000	0.000	1963	0.000	0.000
1964	0.000	0.000	1964	0.000	0.000
1965	0.000	0.000	1965	0.000	0.000
1966	0.000	0.000	1966	0.000	0.000
1967	0.000	0.000	1967	0.000	0.000
1968	0.000	0.000	1968	0.000	0.000
1969	0.000	0.000	1969	0.000	0.000
1970	0.000	0.000	1970	0.000	0.000
1971	0.000	0.000	1971	0.000	0.000
1972	0.000	0.000	1972	0.000	0.000
1973	0.000	0.000	1973	0.000	0.000
1974	0.000	0.000	1974	0.000	0.000
1975	0.000	0.000	1975	0.000	0.000
1976	0.000	0.000	1976	0.000	0.000
1977	0.000	0.000	1977	0.000	0.000
1978	0.000	0.000	1978	0.000	0.000
1979	0.000	0.000	1979	0.000	0.000
1980	0.000	0.000	1980	0.000	0.000
1981	0.000	0.000	1981	0.000	0.000
1982	0.000	0.000	1982	0.000	0.000
1983	0.000	0.000	1983	0.000	0.000
1984	0.000	0.000	1984	0.000	0.000
1985	0.000	0.000	1985	0.000	0.000
1986	0.000	0.000	1986	0.000	0.000
1987	0.000	0.000	1987	0.000	0.000
1988	0.000	0.000	1988	0.000	0.000
1989	0.000	0.000	1989	0.000	0.000
1990	0.000	0.000	1990	0.000	0.000
1991	0.000	0.000	1991	0.000	0.000
1992	0.000	0.000	1992	0.000	0.000
1993	0.000	0.000	1993	0.000	0.000
1994	0.000	0.000	1994	0.000	0.000
1995	0.000	0.000	1995	0.000	0.000
1996	0.000	0.000	1996	0.000	0.000
1997	0.000	0.000	1997	0.000	0.000
1998	0.000	0.000	1998	0.000	0.000
1999	0.000	0.000	1999	0.000	0.000
2000	0.000	0.000	2000	0.000	0.000

TABLE III (Continued)

Rel.			Rel.		
hk ℓ	$\frac{\sin \theta}{\lambda}$	$ F_{hk\ell} ^2$	hk ℓ	$\frac{\sin \theta}{\lambda}$	$ F_{hk\ell} ^2$
22 $\bar{9}$	0.621	21	31 $\bar{1}$	0.292	98
23 $\bar{9}$	0.629	0	32 $\bar{1}$	0.292	800
24 $\bar{9}$	0.637	-	33 $\bar{1}$	0.311	230
			34 $\bar{1}$	0.357	380
300	0.279	169	35 $\bar{1}$	0.422	80
310	0.331	860	36 $\bar{1}$	0.486	70
320	0.389	13	37 $\bar{1}$	0.565	0
330	0.461	98	38 $\bar{1}$	0.630	2
340	0.538	0			
350	0.616	-	302	0.369	110
			312	0.422	53
310	0.259	235	322	0.480	97
320	0.266	162	332	0.545	4.6
330	0.298	26	342	0.617	3.4
340	0.356	580			
350	0.422	30	30 $\bar{2}$	0.266	1600
360	0.493	65	31 $\bar{2}$	0.292	200
370	0.571	35	32 $\bar{2}$	0.350	540
380	0.643	-	33 $\bar{2}$	0.415	24
			34 $\bar{2}$	0.486	64
301	0.318	11	35 $\bar{2}$	0.564	0
311	0.370	9	36 $\bar{2}$	0.636	-
321	0.435	85			
331	0.499	0	312	0.259	52
341	0.570	3.4	322	0.285	150
			332	0.331	120
30 $\bar{1}$	0.266	350	342	0.389	0
31 $\bar{1}$	0.305	230	352	0.467	130
32 $\bar{1}$	0.363	3	362	0.545	0
33 $\bar{1}$	0.435	152	372	0.609	0
34 $\bar{1}$	0.506	13			
35 $\bar{1}$	0.584	28	31 $\bar{2}$	0.337	114
			322	0.331	17.5
311	0.247	37	332	0.344	460
321	0.266	38	342	0.383	270
331	0.305	480	352	0.435	90
341	0.370	120	362	0.493	160
351	0.441	120	372	0.558	4
361	0.512	7.5	382	0.630	14
371	0.596	20			

TABLE III (Continued)

Left			Right		
λ	$\frac{g}{\lambda}$	λ	λ	$\frac{g}{\lambda}$	λ
10	0.000	100	10	0.000	100
20	0.000	200	20	0.000	200
30	0.000	300	30	0.000	300
40	0.000	400	40	0.000	400
50	0.000	500	50	0.000	500
60	0.000	600	60	0.000	600
70	0.000	700	70	0.000	700
80	0.000	800	80	0.000	800
90	0.000	900	90	0.000	900
100	0.000	1000	100	0.000	1000
110	0.000	1100	110	0.000	1100
120	0.000	1200	120	0.000	1200
130	0.000	1300	130	0.000	1300
140	0.000	1400	140	0.000	1400
150	0.000	1500	150	0.000	1500
160	0.000	1600	160	0.000	1600
170	0.000	1700	170	0.000	1700
180	0.000	1800	180	0.000	1800
190	0.000	1900	190	0.000	1900
200	0.000	2000	200	0.000	2000
210	0.000	2100	210	0.000	2100
220	0.000	2200	220	0.000	2200
230	0.000	2300	230	0.000	2300
240	0.000	2400	240	0.000	2400
250	0.000	2500	250	0.000	2500
260	0.000	2600	260	0.000	2600
270	0.000	2700	270	0.000	2700
280	0.000	2800	280	0.000	2800
290	0.000	2900	290	0.000	2900
300	0.000	3000	300	0.000	3000
310	0.000	3100	310	0.000	3100
320	0.000	3200	320	0.000	3200
330	0.000	3300	330	0.000	3300
340	0.000	3400	340	0.000	3400
350	0.000	3500	350	0.000	3500
360	0.000	3600	360	0.000	3600
370	0.000	3700	370	0.000	3700
380	0.000	3800	380	0.000	3800
390	0.000	3900	390	0.000	3900
400	0.000	4000	400	0.000	4000
410	0.000	4100	410	0.000	4100
420	0.000	4200	420	0.000	4200
430	0.000	4300	430	0.000	4300
440	0.000	4400	440	0.000	4400
450	0.000	4500	450	0.000	4500
460	0.000	4600	460	0.000	4600
470	0.000	4700	470	0.000	4700
480	0.000	4800	480	0.000	4800
490	0.000	4900	490	0.000	4900
500	0.000	5000	500	0.000	5000

TABLE III (Continued)

hkl	Rel.		hkl	Rel.	
	$\frac{\sin \theta}{\lambda}$	$(F_{hkl})^2$		$\frac{\sin \theta}{\lambda}$	$(F_{hkl})^2$
303	0.428	34	344	0.486	16
313	0.473	4.5	354	0.558	0
323	0.533	4.5	364	0.629	-
333	0.597	2.7			
$\bar{3}0\bar{3}$	0.285	150	$\bar{3}14$	0.337	1525
$\bar{3}1\bar{3}$	0.311	45	$\bar{3}24$	0.370	4
$\bar{3}2\bar{3}$	0.350	640	$\bar{3}34$	0.421	10
$\bar{3}3\bar{3}$	0.415	30	$\bar{3}44$	0.480	30
$\bar{3}4\bar{3}$	0.487	228	$\bar{3}54$	0.551	1.5
$\bar{3}5\bar{3}$	0.558	26	$\bar{3}64$	0.623	8
$\bar{3}6\bar{3}$	0.629	-			
$\bar{3}1\bar{3}$	0.292	530	$\bar{3}1\bar{4}$	0.461	3.2
$\bar{3}2\bar{3}$	0.324	15	$\bar{3}2\bar{4}$	0.441	125
$\bar{3}3\bar{3}$	0.370	21	$\bar{3}3\bar{4}$	0.441	130
$\bar{3}4\bar{3}$	0.435	48	$\bar{3}4\bar{4}$	0.461	0
$\bar{3}5\bar{3}$	0.506	33	$\bar{3}5\bar{4}$	0.493	140
$\bar{3}6\bar{3}$	0.577	0	$\bar{3}6\bar{4}$	0.538	0
$\bar{3}7\bar{3}$	0.654	0	$\bar{3}7\bar{4}$	0.591	11
$\bar{3}1\bar{3}$	0.396	334	305	0.558	26
$\bar{3}2\bar{3}$	0.383	60	315	0.603	8
$\bar{3}3\bar{3}$	0.389	130			
$\bar{3}4\bar{3}$	0.415	45	305	0.383	10
$\bar{3}5\bar{3}$	0.454	0	315	0.389	300
$\bar{3}6\bar{3}$	0.512	40	325	0.409	36
$\bar{3}7\bar{3}$	0.571	0	335	0.454	558
$\bar{3}8\bar{3}$	0.637	-	345	0.506	114
-			355	0.571	0
			365	0.636	-
304	0.493	36	$\bar{3}15$	0.395	2.9
314	0.538	12	$\bar{3}25$	0.435	170
324	0.597	2	$\bar{3}35$	0.480	0
			$\bar{3}45$	0.538	0
$\bar{3}0\bar{4}$	0.331	200	$\bar{3}55$	0.598	2.3
$\bar{3}1\bar{4}$	0.337	800			
$\bar{3}2\bar{4}$	0.376	128	$\bar{3}15$	0.532	3.9
$\bar{3}3\bar{4}$	0.428	135	$\bar{3}25$	0.513	12
			$\bar{3}35$	0.506	0
			$\bar{3}45$	0.513	14
			$\bar{3}55$	0.538	0

Year	Price	Quantity	Year	Price	Quantity
1910	100.0	100	1911	100.0	100
1912	100.0	100	1913	100.0	100
1914	100.0	100	1915	100.0	100
1916	100.0	100	1917	100.0	100
1918	100.0	100	1919	100.0	100
1920	100.0	100	1921	100.0	100
1922	100.0	100	1923	100.0	100
1924	100.0	100	1925	100.0	100
1926	100.0	100	1927	100.0	100
1928	100.0	100	1929	100.0	100
1930	100.0	100	1931	100.0	100
1932	100.0	100	1933	100.0	100
1934	100.0	100	1935	100.0	100
1936	100.0	100	1937	100.0	100
1938	100.0	100	1939	100.0	100
1940	100.0	100	1941	100.0	100
1942	100.0	100	1943	100.0	100
1944	100.0	100	1945	100.0	100
1946	100.0	100	1947	100.0	100
1948	100.0	100	1949	100.0	100
1950	100.0	100	1951	100.0	100
1952	100.0	100	1953	100.0	100
1954	100.0	100	1955	100.0	100
1956	100.0	100	1957	100.0	100
1958	100.0	100	1959	100.0	100
1960	100.0	100	1961	100.0	100
1962	100.0	100	1963	100.0	100
1964	100.0	100	1965	100.0	100
1966	100.0	100	1967	100.0	100
1968	100.0	100	1969	100.0	100
1970	100.0	100	1971	100.0	100
1972	100.0	100	1973	100.0	100
1974	100.0	100	1975	100.0	100
1976	100.0	100	1977	100.0	100
1978	100.0	100	1979	100.0	100
1980	100.0	100	1981	100.0	100
1982	100.0	100	1983	100.0	100
1984	100.0	100	1985	100.0	100
1986	100.0	100	1987	100.0	100
1988	100.0	100	1989	100.0	100
1990	100.0	100	1991	100.0	100
1992	100.0	100	1993	100.0	100
1994	100.0	100	1995	100.0	100
1996	100.0	100	1997	100.0	100
1998	100.0	100	1999	100.0	100
2000	100.0	100	2001	100.0	100
2002	100.0	100	2003	100.0	100
2004	100.0	100	2005	100.0	100
2006	100.0	100	2007	100.0	100
2008	100.0	100	2009	100.0	100
2010	100.0	100	2011	100.0	100
2012	100.0	100	2013	100.0	100
2014	100.0	100	2015	100.0	100
2016	100.0	100	2017	100.0	100
2018	100.0	100	2019	100.0	100
2020	100.0	100	2021	100.0	100
2022	100.0	100	2023	100.0	100
2024	100.0	100	2025	100.0	100

TABLE III (Continued)

Rel.			Rel.		
hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$	hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$
$\bar{3}65$	0.577	0	$30\bar{9}$	0.577	0
$\bar{3}75$	0.623	1.8	$31\bar{8}$	0.571	2.4
306	0.629	0	$32\bar{8}$	0.571	2.4
$30\bar{6}$	0.441	320	$33\bar{8}$	0.584	0
$31\bar{6}$	0.441	45	$34\bar{8}$	0.616	0
$32\bar{6}$	0.454	51	$\bar{3}18$	0.596	5.4
$33\bar{6}$	0.486	24	$\bar{3}28$	0.630	6.8
$34\bar{6}$	0.532	20	$30\bar{9}$	0.641	1.3
$35\bar{6}$	0.590	9.5	$31\bar{9}$	0.630	4.1
$36\bar{6}$	0.648	-	$32\bar{9}$	0.630	1.3
$\bar{3}16$	0.461	115	$33\bar{9}$	0.641	14
$\bar{3}26$	0.493	280	400	0.376	130
$\bar{3}36$	0.538	14.5	410	0.422	13
$\bar{3}46$	0.597	0	420	0.473	90
$\bar{3}56$	0.650	0.1	430	0.538	0
$\bar{3}1\bar{6}$	0.597	6.2	440	0.610	1.1
$\bar{3}2\bar{6}$	0.571	2.8	$\bar{4}10$	0.350	300
$\bar{3}3\bar{6}$	0.564	9.4	$\bar{4}20$	0.350	210
$\bar{3}4\bar{6}$	0.571	17	$\bar{4}30$	0.363	400
$\bar{3}5\bar{6}$	0.591	0	$\bar{4}40$	0.402	90
366	0.616	10	$\bar{4}50$	0.454	25
$30\bar{7}$	0.506	45	$\bar{4}60$	0.512	0
$31\bar{7}$	0.499	17.5	$\bar{4}70$	0.577	0
$32\bar{7}$	0.512	145	401	0.408	75
$33\bar{7}$	0.532	21.8	411	0.454	84
$34\bar{7}$	0.571	6.1	421	0.519	77
$35\bar{7}$	0.616	14.8	431	0.577	0
$\bar{3}17$	0.525	32	$40\bar{1}$	0.357	80
$\bar{3}27$	0.558	16	$41\bar{1}$	0.389	310
$\bar{3}37$	0.610	9.5	$42\bar{1}$	0.447	90
$\bar{3}2\bar{7}$	0.642	-	$43\bar{1}$	0.512	0
$\bar{3}3\bar{7}$	0.629	-	$44\bar{1}$	0.578	4.1
$\bar{3}4\bar{7}$	0.629	-	$\bar{4}11$	0.337	80
$\bar{3}5\bar{7}$	0.642	-	$\bar{4}21$	0.337	500

(Continued) Table 111

Year	1960	1961	1962	1963	1964
0	172.0	172.0	172.0	172.0	172.0
1	172.0	172.0	172.0	172.0	172.0
2	172.0	172.0	172.0	172.0	172.0
3	172.0	172.0	172.0	172.0	172.0
4	172.0	172.0	172.0	172.0	172.0
5	172.0	172.0	172.0	172.0	172.0
6	172.0	172.0	172.0	172.0	172.0
7	172.0	172.0	172.0	172.0	172.0
8	172.0	172.0	172.0	172.0	172.0
9	172.0	172.0	172.0	172.0	172.0
10	172.0	172.0	172.0	172.0	172.0
11	172.0	172.0	172.0	172.0	172.0
12	172.0	172.0	172.0	172.0	172.0
13	172.0	172.0	172.0	172.0	172.0
14	172.0	172.0	172.0	172.0	172.0
15	172.0	172.0	172.0	172.0	172.0
16	172.0	172.0	172.0	172.0	172.0
17	172.0	172.0	172.0	172.0	172.0
18	172.0	172.0	172.0	172.0	172.0
19	172.0	172.0	172.0	172.0	172.0
20	172.0	172.0	172.0	172.0	172.0
21	172.0	172.0	172.0	172.0	172.0
22	172.0	172.0	172.0	172.0	172.0
23	172.0	172.0	172.0	172.0	172.0
24	172.0	172.0	172.0	172.0	172.0
25	172.0	172.0	172.0	172.0	172.0
26	172.0	172.0	172.0	172.0	172.0
27	172.0	172.0	172.0	172.0	172.0
28	172.0	172.0	172.0	172.0	172.0
29	172.0	172.0	172.0	172.0	172.0
30	172.0	172.0	172.0	172.0	172.0
31	172.0	172.0	172.0	172.0	172.0
32	172.0	172.0	172.0	172.0	172.0
33	172.0	172.0	172.0	172.0	172.0
34	172.0	172.0	172.0	172.0	172.0
35	172.0	172.0	172.0	172.0	172.0
36	172.0	172.0	172.0	172.0	172.0
37	172.0	172.0	172.0	172.0	172.0
38	172.0	172.0	172.0	172.0	172.0
39	172.0	172.0	172.0	172.0	172.0
40	172.0	172.0	172.0	172.0	172.0
41	172.0	172.0	172.0	172.0	172.0
42	172.0	172.0	172.0	172.0	172.0
43	172.0	172.0	172.0	172.0	172.0
44	172.0	172.0	172.0	172.0	172.0
45	172.0	172.0	172.0	172.0	172.0
46	172.0	172.0	172.0	172.0	172.0
47	172.0	172.0	172.0	172.0	172.0
48	172.0	172.0	172.0	172.0	172.0
49	172.0	172.0	172.0	172.0	172.0
50	172.0	172.0	172.0	172.0	172.0

TABLE III (Continued)

Rel.			Rel.		
hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$	hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$
$\bar{4}31$	0.363	34	$\bar{4}8\bar{2}$	0.648	-
$\bar{4}41$	0.402	15	403	0.512	9.1
$\bar{4}51$	0.461	130	413	0.558	0
$\bar{4}61$	0.525	0	423	0.596	8.9
$\bar{4}71$	0.596	15	40 $\bar{3}$	0.357	48
41 $\bar{1}$	0.383	115	41 $\bar{3}$	0.383	160
42 $\bar{1}$	0.376	90	42 $\bar{3}$	0.428	123
43 $\bar{1}$	0.383	6	43 $\bar{3}$	0.486	19
44 $\bar{1}$	0.408	190	44 $\bar{3}$	0.551	0
45 $\bar{1}$	0.454	10	45 $\bar{3}$	0.623	-
46 $\bar{1}$	0.512	70	413	0.357	185
47 $\bar{1}$	0.577	0	423	0.369	160
402	0.461	86	433	0.402	125
412	0.506	42	443	0.454	0
422	0.564	20	453	0.512	18
432	0.623	7	463	0.577	18
40 $\bar{2}$	0.350	34	473	0.647	-
41 $\bar{2}$	0.382	76	41 $\bar{3}$	0.480	38
42 $\bar{2}$	0.435	12	42 $\bar{3}$	0.461	2.5
43 $\bar{2}$	0.493	27	43 $\bar{3}$	0.461	65
44 $\bar{2}$	0.558	12.3	44 $\bar{3}$	0.473	20
45 $\bar{2}$	0.636	-	45 $\bar{3}$	0.499	50
412	0.337	6.5	46 $\bar{3}$	0.545	0
422	0.344	600	47 $\bar{3}$	0.597	7.5
432	0.376	260	404	0.571	0
442	0.422	400	414	0.616	5
452	0.480	80	40 $\bar{4}$	0.383	115
462	0.545	4.5	41 $\bar{4}$	0.402	305
472	0.592	0	42 $\bar{4}$	0.441	14.5
41 $\bar{2}$	0.428	26	43 $\bar{4}$	0.487	86
42 $\bar{2}$	0.408	170	44 $\bar{4}$	0.551	18
43 $\bar{2}$	0.415	3	45 $\bar{4}$	0.616	-
44 $\bar{2}$	0.434	22	414	0.383	58
45 $\bar{2}$	0.473	0	424	0.402	20
46 $\bar{2}$	0.525	10.8			
472	0.584	13.3			

What is the purpose of the study?

Year	Q. 1st	Q. 2nd	Q. 3rd	Q. 4th	Year	Q. 1st	Q. 2nd	Q. 3rd	Q. 4th
-	0.000	0.000	0.000	0.000	1900	0.000	0.000	0.000	0.000
1.0	0.000	0.000	0.000	0.000	1901	0.000	0.000	0.000	0.000
2.0	0.000	0.000	0.000	0.000	1902	0.000	0.000	0.000	0.000
3.0	0.000	0.000	0.000	0.000	1903	0.000	0.000	0.000	0.000
4.0	0.000	0.000	0.000	0.000	1904	0.000	0.000	0.000	0.000
5.0	0.000	0.000	0.000	0.000	1905	0.000	0.000	0.000	0.000
6.0	0.000	0.000	0.000	0.000	1906	0.000	0.000	0.000	0.000
7.0	0.000	0.000	0.000	0.000	1907	0.000	0.000	0.000	0.000
8.0	0.000	0.000	0.000	0.000	1908	0.000	0.000	0.000	0.000
9.0	0.000	0.000	0.000	0.000	1909	0.000	0.000	0.000	0.000
10.0	0.000	0.000	0.000	0.000	1910	0.000	0.000	0.000	0.000
11.0	0.000	0.000	0.000	0.000	1911	0.000	0.000	0.000	0.000
12.0	0.000	0.000	0.000	0.000	1912	0.000	0.000	0.000	0.000
13.0	0.000	0.000	0.000	0.000	1913	0.000	0.000	0.000	0.000
14.0	0.000	0.000	0.000	0.000	1914	0.000	0.000	0.000	0.000
15.0	0.000	0.000	0.000	0.000	1915	0.000	0.000	0.000	0.000
16.0	0.000	0.000	0.000	0.000	1916	0.000	0.000	0.000	0.000
17.0	0.000	0.000	0.000	0.000	1917	0.000	0.000	0.000	0.000
18.0	0.000	0.000	0.000	0.000	1918	0.000	0.000	0.000	0.000
19.0	0.000	0.000	0.000	0.000	1919	0.000	0.000	0.000	0.000
20.0	0.000	0.000	0.000	0.000	1920	0.000	0.000	0.000	0.000

TABLE III (Continued)

Rel.			Rel.		
hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$	hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$
$\bar{4}34$	0.441	283	$\bar{4}16$	0.479	135
$\bar{4}44$	0.493	63	$\bar{4}26$	0.506	0
$\bar{4}54$	0.551	55	$\bar{4}36$	0.545	29
$\bar{4}64$	0.596	8.1	$\bar{4}46$	0.596	7.8
$\bar{4}1\bar{4}$	0.538	12.5	$\bar{4}2\bar{5}$	0.636	-
$\bar{4}2\bar{4}$	0.519	6.7	$\bar{4}3\bar{5}$	0.630	-
$\bar{4}3\bar{4}$	0.506	0	$\bar{4}4\bar{5}$	0.623	2.1
$\bar{4}4\bar{4}$	0.519	2.3	$\bar{4}5\bar{5}$	0.636	0
$\bar{4}5\bar{4}$	0.538	0			
$\bar{4}6\bar{4}$	0.577	0	$40\bar{7}$	0.525	21
$\bar{4}7\bar{4}$	0.623	0	$41\bar{7}$	0.525	0
			$42\bar{7}$	0.538	8.3
405	0.636	3	$43\bar{7}$	0.571	17
			$44\bar{7}$	0.609	6
$40\bar{5}$	0.422	4.5			
$41\bar{5}$	0.434	190	$\bar{4}17$	0.538	7.5
$42\bar{5}$	0.461	4	$\bar{4}27$	0.564	42
$43\bar{5}$	0.506	0	$\bar{4}37$	0.603	1.6
$44\bar{5}$	0.558	10			
$45\bar{5}$	0.623	-	$40\bar{8}$	0.584	9
			$41\bar{8}$	0.594	32
$\bar{4}15$	0.428	53	$42\bar{8}$	0.590	3.2
$\bar{4}25$	0.448	160	$43\bar{8}$	0.616	15.5
$\bar{4}35$	0.493	39	$44\bar{8}$	0.649	3.2
$\bar{4}45$	0.545	2.5			
$\bar{4}55$	0.598	-	$\bar{4}18$	0.591	0
			$\bar{4}28$	0.630	1.5
$\bar{4}1\bar{5}$	0.597	0			
$\bar{4}2\bar{5}$	0.577	10	$40\bar{9}$	0.592	0
$\bar{4}3\bar{5}$	0.564	11	$41\bar{9}$	0.649	2.3
$\bar{4}4\bar{5}$	0.571	35	$42\bar{9}$	0.636	-
$\bar{4}5\bar{5}$	0.584	0	$43\bar{9}$	0.649	-
$\bar{4}6\bar{5}$	0.616	0			
			$\bar{4}19$	0.649	0.6
$40\bar{6}$	0.467	130			
$41\bar{6}$	0.473	21	500	0.472	90
$42\bar{6}$	0.499	109	510	0.514	53.3
$43\bar{6}$	0.532	11.5	520	0.565	0
$44\bar{6}$	0.577	0	530	0.623	0
$45\bar{6}$	0.636	-			

TABLE III (Continued)

hkl	Rel.		hkl	Rel.	
	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$		$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$
510	0.448	4.5	512	0.416	174
520	0.435	7.1	522	0.416	120
530	0.435	160	532	0.435	19
540	0.467	634	542	0.474	50
550	0.505	14.9	552	0.518	276
560	0.552	31.4	562	0.578	7
570	0.611	3.1	572	0.637	0
501	0.506	0	51 $\bar{2}$	0.520	0
511	0.552	0	52 $\bar{2}$	0.500	41
521	0.611	0	53 $\bar{2}$	0.493	240
50 $\bar{1}$	0.447	4	54 $\bar{2}$	0.506	0
51 $\bar{1}$	0.487	184	55 $\bar{2}$	0.537	4.1
52 $\bar{1}$	0.539	3	56 $\bar{2}$	0.572	0
53 $\bar{1}$	0.598	11.2	57 $\bar{2}$	0.624	-
511	0.422	90	503	0.601	2
521	0.416	16	513	0.643	0
531	0.429	195	50 $\bar{3}$	0.443	563
541	0.461	49	51 $\bar{3}$	0.461	8.1
551	0.505	26.6	52 $\bar{3}$	0.507	72.9
561	0.559	10.1	53 $\bar{3}$	0.559	0
571	0.617	0	54 $\bar{3}$	0.623	0
51 $\bar{1}$	0.474	28	513	0.422	278
52 $\bar{1}$	0.461	54	523	0.429	123
53 $\bar{1}$	0.461	16	533	0.455	21
54 $\bar{1}$	0.481	72	543	0.493	40
55 $\bar{1}$	0.516	0	553	0.542	19
56 $\bar{1}$	0.559	16.7	563	0.598	6.8
57 $\bar{1}$	0.611	38.1	51 $\bar{3}$	0.565	7.7
502	0.550	0	52 $\bar{3}$	0.546	0
512	0.598	0	53 $\bar{3}$	0.533	25
50 $\bar{2}$	0.433	18	54 $\bar{3}$	0.539	0
512	0.467	31	55 $\bar{3}$	0.571	18.8
522	0.520	33	56 $\bar{3}$	0.598	-
532	0.572	16	57 $\bar{3}$	0.640	-
542	0.637	-	534	0.559	0

(continued) TEST DATA

Test	Test	Test	Test	Test	Test
λ_{opt}	$\frac{v_{opt}}{\lambda}$	λ_{opt}	λ_{opt}	$\frac{v_{opt}}{\lambda}$	λ_{opt}
0.1	0.14, 0	0.14	0.14	0.14, 0	0.14
0.2	0.28, 0	0.28	0.28	0.28, 0	0.28
0.3	0.42, 0	0.42	0.42	0.42, 0	0.42
0.4	0.56, 0	0.56	0.56	0.56, 0	0.56
0.5	0.70, 0	0.70	0.70	0.70, 0	0.70
0.6	0.84, 0	0.84	0.84	0.84, 0	0.84
0.7	0.98, 0	0.98	0.98	0.98, 0	0.98
0.8	1.12, 0	1.12	1.12	1.12, 0	1.12
0.9	1.26, 0	1.26	1.26	1.26, 0	1.26
1.0	1.40, 0	1.40	1.40	1.40, 0	1.40
1.1	1.54, 0	1.54	1.54	1.54, 0	1.54
1.2	1.68, 0	1.68	1.68	1.68, 0	1.68
1.3	1.82, 0	1.82	1.82	1.82, 0	1.82
1.4	1.96, 0	1.96	1.96	1.96, 0	1.96
1.5	2.10, 0	2.10	2.10	2.10, 0	2.10
1.6	2.24, 0	2.24	2.24	2.24, 0	2.24
1.7	2.38, 0	2.38	2.38	2.38, 0	2.38
1.8	2.52, 0	2.52	2.52	2.52, 0	2.52
1.9	2.66, 0	2.66	2.66	2.66, 0	2.66
2.0	2.80, 0	2.80	2.80	2.80, 0	2.80
2.1	2.94, 0	2.94	2.94	2.94, 0	2.94
2.2	3.08, 0	3.08	3.08	3.08, 0	3.08
2.3	3.22, 0	3.22	3.22	3.22, 0	3.22
2.4	3.36, 0	3.36	3.36	3.36, 0	3.36
2.5	3.50, 0	3.50	3.50	3.50, 0	3.50
2.6	3.64, 0	3.64	3.64	3.64, 0	3.64
2.7	3.78, 0	3.78	3.78	3.78, 0	3.78
2.8	3.92, 0	3.92	3.92	3.92, 0	3.92
2.9	4.06, 0	4.06	4.06	4.06, 0	4.06
3.0	4.20, 0	4.20	4.20	4.20, 0	4.20
3.1	4.34, 0	4.34	4.34	4.34, 0	4.34
3.2	4.48, 0	4.48	4.48	4.48, 0	4.48
3.3	4.62, 0	4.62	4.62	4.62, 0	4.62
3.4	4.76, 0	4.76	4.76	4.76, 0	4.76
3.5	4.90, 0	4.90	4.90	4.90, 0	4.90
3.6	5.04, 0	5.04	5.04	5.04, 0	5.04
3.7	5.18, 0	5.18	5.18	5.18, 0	5.18
3.8	5.32, 0	5.32	5.32	5.32, 0	5.32
3.9	5.46, 0	5.46	5.46	5.46, 0	5.46
4.0	5.60, 0	5.60	5.60	5.60, 0	5.60

TABLE III (Continued)

Rel.			Rel.		
hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$	hkl	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$
504	0.447	380	516	0.513	130
514	0.474	103	526	0.533	21
524	0.510	165	536	0.565	8
534	0.559	0	546	0.611	0
544	0.617	0			
			507	0.551	0
514	0.442	0	517	0.558	0
524	0.455	2.5	527	0.584	-
534	0.481	60	537	0.611	-
544	0.520	3			
554	0.575	6	517	0.558	0
564	0.637	0	527	0.585	7.5
			537	0.617	2.2
514	0.618	3			
524	0.580	44	508	0.601	14
534	0.624	0.8	518	0.603	-
544	0.580	0	528	0.624	0
554	0.609	0	538	0.646	-
564	0.630	-			
			518	0.617	0
505	0.473	21	528	0.643	0
515	0.494	16.5			
525	0.525	0	600	0.565	6.3
535	0.565	-	610	0.604	3.6
545	0.617	8.7			
			610	0.539	0
515	0.474	95	620	0.519	3.2
525	0.490	148	630	0.520	0
535	0.520	18	640	0.533	0
545	0.565	16	650	0.572	4.5
555	0.613	3.5	660	0.607	7.6
535	0.636	4	601	0.600	6.3
545	0.636	3.6	611	0.643	0
506	0.508	1	601	0.540	9.3
516	0.520	200	611	0.578	10.9
526	0.545	0	621	0.630	-
536	0.585	-			
546	0.630	-	611	0.513	60
			621	0.506	152

TABLE III (Continued)

hkl	$\frac{\sin \theta}{\lambda}$	Rel.	hkl	$\frac{\sin \theta}{\lambda}$	Rel.
		$ F_{hkl} ^2$			$ F_{hkl} ^2$
$\bar{5}31$	0.506	0	$\bar{5}53$	0.591	7
$\bar{6}41$	0.526	0	$\bar{6}33$	0.615	5
$\bar{6}51$	0.565	12	$\bar{6}53$	0.600	3
$\bar{6}61$	0.603	0	$\bar{6}63$	0.633	17
$\bar{6}1\bar{1}$	0.565	40	$60\bar{4}$	0.524	2.8
$\bar{6}2\bar{1}$	0.552	0	$61\bar{2}$	0.552	0
$\bar{6}3\bar{1}$	0.552	1.7	$62\bar{4}$	0.592	-
$\bar{6}4\bar{1}$	0.552	2.5	$63\bar{4}$	0.636	12
$\bar{6}5\bar{1}$	0.585	8	$\bar{6}14$	0.513	6.5
$\bar{6}6\bar{1}$	0.615	5	$\bar{6}24$	0.519	102
602	0.640	0	$\bar{6}34$	0.532	3.5
$60\bar{2}$	0.524	0	$\bar{6}44$	0.565	0
$61\bar{2}$	0.558	0	$\bar{6}54$	0.611	0
$62\bar{2}$	0.611	0	$60\bar{5}$	0.540	0
$\bar{6}12$	0.500	90	$61\bar{5}$	0.565	0
$\bar{6}22$	0.500	0	$62\bar{5}$	0.598	-
$\bar{6}32$	0.506	0	$63\bar{5}$	0.636	-
$\bar{6}42$	0.529	0	$\bar{6}15$	0.532	0
$\bar{6}52$	0.572	8.9	$\bar{6}25$	0.546	8.6
$\bar{6}62$	0.613	0	$\bar{6}35$	0.565	2.5
$\bar{6}1\bar{2}$	0.604	2.4	$\bar{6}45$	0.597	15
$\bar{6}2\bar{2}$	0.592	-	$60\bar{6}$	0.566	1
$\bar{6}3\bar{2}$	0.578	-	$61\bar{6}$	0.585	0
$\bar{6}4\bar{2}$	0.581	2.6	$62\bar{6}$	0.617	-
$\bar{6}5\bar{2}$	0.591	0	$63\bar{6}$	0.649	-
$\bar{6}6\bar{2}$	0.635	0	$\bar{6}16$	0.565	5
$60\bar{3}$	0.518	4.9	$\bar{6}26$	0.578	0
$61\bar{3}$	0.552	0	$\bar{6}36$	0.604	9
$62\bar{3}$	0.593	0	$\bar{6}46$	0.640	0
$63\bar{3}$	0.643	4	$60\bar{7}$	0.601	2.6
$\bar{6}13$	0.500	50	$61\bar{7}$	0.617	-
$\bar{6}23$	0.500	20	$62\bar{7}$	0.647	-
$\bar{6}33$	0.513	138			
$\bar{6}43$	0.546	10			

TABLE III (Continued)

Left			Right		
λ	$\frac{P_{010}}{\lambda}$	λ	λ	$\frac{P_{010}}{\lambda}$	λ
1	0.000	100	0	0.000	100
2	0.000	100	0	0.000	100
3	0.000	100	0	0.000	100
4	0.000	100	0	0.000	100
5	0.000	100	0	0.000	100
6	0.000	100	0	0.000	100
7	0.000	100	0	0.000	100
8	0.000	100	0	0.000	100
9	0.000	100	0	0.000	100
10	0.000	100	0	0.000	100
11	0.000	100	0	0.000	100
12	0.000	100	0	0.000	100
13	0.000	100	0	0.000	100
14	0.000	100	0	0.000	100
15	0.000	100	0	0.000	100
16	0.000	100	0	0.000	100
17	0.000	100	0	0.000	100
18	0.000	100	0	0.000	100
19	0.000	100	0	0.000	100
20	0.000	100	0	0.000	100
21	0.000	100	0	0.000	100
22	0.000	100	0	0.000	100
23	0.000	100	0	0.000	100
24	0.000	100	0	0.000	100
25	0.000	100	0	0.000	100
26	0.000	100	0	0.000	100
27	0.000	100	0	0.000	100
28	0.000	100	0	0.000	100
29	0.000	100	0	0.000	100
30	0.000	100	0	0.000	100
31	0.000	100	0	0.000	100
32	0.000	100	0	0.000	100
33	0.000	100	0	0.000	100
34	0.000	100	0	0.000	100
35	0.000	100	0	0.000	100
36	0.000	100	0	0.000	100
37	0.000	100	0	0.000	100
38	0.000	100	0	0.000	100
39	0.000	100	0	0.000	100
40	0.000	100	0	0.000	100
41	0.000	100	0	0.000	100
42	0.000	100	0	0.000	100
43	0.000	100	0	0.000	100
44	0.000	100	0	0.000	100
45	0.000	100	0	0.000	100
46	0.000	100	0	0.000	100
47	0.000	100	0	0.000	100
48	0.000	100	0	0.000	100
49	0.000	100	0	0.000	100
50	0.000	100	0	0.000	100
51	0.000	100	0	0.000	100
52	0.000	100	0	0.000	100
53	0.000	100	0	0.000	100
54	0.000	100	0	0.000	100
55	0.000	100	0	0.000	100
56	0.000	100	0	0.000	100
57	0.000	100	0	0.000	100
58	0.000	100	0	0.000	100
59	0.000	100	0	0.000	100
60	0.000	100	0	0.000	100
61	0.000	100	0	0.000	100
62	0.000	100	0	0.000	100
63	0.000	100	0	0.000	100
64	0.000	100	0	0.000	100
65	0.000	100	0	0.000	100
66	0.000	100	0	0.000	100
67	0.000	100	0	0.000	100
68	0.000	100	0	0.000	100
69	0.000	100	0	0.000	100
70	0.000	100	0	0.000	100
71	0.000	100	0	0.000	100
72	0.000	100	0	0.000	100
73	0.000	100	0	0.000	100
74	0.000	100	0	0.000	100
75	0.000	100	0	0.000	100
76	0.000	100	0	0.000	100
77	0.000	100	0	0.000	100
78	0.000	100	0	0.000	100
79	0.000	100	0	0.000	100
80	0.000	100	0	0.000	100
81	0.000	100	0	0.000	100
82	0.000	100	0	0.000	100
83	0.000	100	0	0.000	100
84	0.000	100	0	0.000	100
85	0.000	100	0	0.000	100
86	0.000	100	0	0.000	100
87	0.000	100	0	0.000	100
88	0.000	100	0	0.000	100
89	0.000	100	0	0.000	100
90	0.000	100	0	0.000	100
91	0.000	100	0	0.000	100
92	0.000	100	0	0.000	100
93	0.000	100	0	0.000	100
94	0.000	100	0	0.000	100
95	0.000	100	0	0.000	100
96	0.000	100	0	0.000	100
97	0.000	100	0	0.000	100
98	0.000	100	0	0.000	100
99	0.000	100	0	0.000	100
100	0.000	100	0	0.000	100

TABLE III (Continued)

hkl	Rel.		hkl	Rel.	
	$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$		$\frac{\sin \theta}{\lambda}$	$ F_{hkl} ^2$
$\bar{6}17$	0.604	0	$70\bar{3}$	0.606	6.5
$\bar{6}27$	0.624	6.3	$71\bar{3}$	0.637	52.6
$\bar{6}37$	0.646	-	$74\bar{3}$	0.618	17
$60\bar{8}$	0.641	0	$\bar{7}13$	0.618	17
$\bar{6}18$	0.649	-	$\bar{7}23$	0.585	0
750	0.636	24.8	$\bar{7}33$	0.585	14
$\bar{7}30$	0.610	15	$\bar{7}43$	0.585	3.2
$70\bar{1}$	0.634	0	$\bar{7}53$	0.604	12
$\bar{7}11$	0.604	0	$70\bar{4}$	0.606	19
$\bar{7}21$	0.598	5	$71\bar{4}$	0.633	-
$\bar{7}31$	0.591	7	$\bar{7}14$	0.591	18.9
$\bar{7}41$	0.604	0	$\bar{7}24$	0.591	4
$\bar{7}51$	0.622	14	$\bar{7}34$	0.604	10
$\bar{7}3\bar{1}$	0.630	0	$70\bar{5}$	0.615	48.7
$70\bar{2}$	0.615	13.3	$75\bar{1}$	0.640	-
$\bar{7}12$	0.591	0	$\bar{7}15$	0.604	10.6
$\bar{7}22$	0.585	0	$\bar{7}25$	0.610	0
$\bar{7}32$	0.585	0	$\bar{7}35$	0.623	0
$\bar{7}42$	0.597	0	$\bar{7}45$	0.649	0
			$70\bar{6}$	0.633	2.9
			$\bar{7}16$	0.627	38.4
			$\bar{7}26$	0.637	25.0

The factors by which relative F^2 values of a given film were multiplied to reach the common level are:

TABLE III (Continued)

Year	Relative $\frac{W}{A}$	Year	Relative $\frac{W}{A}$	Year
1917	0.000	1927	0.000	1937
1918	0.000	1928	0.000	1938
1919	0.000	1929	0.000	1939
1920	0.000	1930	0.000	1940
1921	0.000	1931	0.000	1941
1922	0.000	1932	0.000	1942
1923	0.000	1933	0.000	1943
1924	0.000	1934	0.000	1944
1925	0.000	1935	0.000	1945
1926	0.000	1936	0.000	1946
1927	0.000	1937	0.000	1947
1928	0.000	1938	0.000	1948
1929	0.000	1939	0.000	1949
1930	0.000	1940	0.000	1950
1931	0.000	1941	0.000	1951
1932	0.000	1942	0.000	1952
1933	0.000	1943	0.000	1953
1934	0.000	1944	0.000	1954
1935	0.000	1945	0.000	1955
1936	0.000	1946	0.000	1956
1937	0.000	1947	0.000	1957
1938	0.000	1948	0.000	1958
1939	0.000	1949	0.000	1959
1940	0.000	1950	0.000	1960
1941	0.000	1951	0.000	1961
1942	0.000	1952	0.000	1962
1943	0.000	1953	0.000	1963
1944	0.000	1954	0.000	1964
1945	0.000	1955	0.000	1965
1946	0.000	1956	0.000	1966
1947	0.000	1957	0.000	1967
1948	0.000	1958	0.000	1968
1949	0.000	1959	0.000	1969
1950	0.000	1960	0.000	1970
1951	0.000	1961	0.000	1971
1952	0.000	1962	0.000	1972
1953	0.000	1963	0.000	1973
1954	0.000	1964	0.000	1974
1955	0.000	1965	0.000	1975
1956	0.000	1966	0.000	1976
1957	0.000	1967	0.000	1977
1958	0.000	1968	0.000	1978
1959	0.000	1969	0.000	1979
1960	0.000	1970	0.000	1980
1961	0.000	1971	0.000	1981
1962	0.000	1972	0.000	1982
1963	0.000	1973	0.000	1983
1964	0.000	1974	0.000	1984
1965	0.000	1975	0.000	1985
1966	0.000	1976	0.000	1986
1967	0.000	1977	0.000	1987
1968	0.000	1978	0.000	1988
1969	0.000	1979	0.000	1989
1970	0.000	1980	0.000	1990
1971	0.000	1981	0.000	1991
1972	0.000	1982	0.000	1992
1973	0.000	1983	0.000	1993
1974	0.000	1984	0.000	1994
1975	0.000	1985	0.000	1995
1976	0.000	1986	0.000	1996
1977	0.000	1987	0.000	1997
1978	0.000	1988	0.000	1998
1979	0.000	1989	0.000	1999
1980	0.000	1990	0.000	2000
1981	0.000	1991	0.000	2001
1982	0.000	1992	0.000	2002
1983	0.000	1993	0.000	2003
1984	0.000	1994	0.000	2004
1985	0.000	1995	0.000	2005
1986	0.000	1996	0.000	2006
1987	0.000	1997	0.000	2007
1988	0.000	1998	0.000	2008
1989	0.000	1999	0.000	2009
1990	0.000	2000	0.000	2010
1991	0.000	2001	0.000	2011
1992	0.000	2002	0.000	2012
1993	0.000	2003	0.000	2013
1994	0.000	2004	0.000	2014
1995	0.000	2005	0.000	2015
1996	0.000	2006	0.000	2016
1997	0.000	2007	0.000	2017
1998	0.000	2008	0.000	2018
1999	0.000	2009	0.000	2019
2000	0.000	2010	0.000	2020

The factors of which relative $\frac{W}{A}$ values of a given item were multiplied to reach the common level are:

<u>Axis</u>	<u>Layer</u>	<u>Factor</u>	<u>Axis</u>	<u>Layer</u>	<u>Factor</u>
a_1	1	1.20	a_3''	0	2.05
	2	0.99		1	2.35
	3	1.05		2	2.56
	4	1.46		3	2.78
a_2	0	0.56		4	2.55
	1	0.91		5	3.04
	2	1.29			
	3	1.32			
	4	1.62			

Absorption effects were calculated to be negligible.

Case	Factor	Level	Value	Factor	Level	Value
1	1.75	1	0.0	1	1	0.0
2	0.99	2	0.0	2	2	0.0
3	1.05	3	0.0	3	3	0.0
4	1.15	4	0.0	4	4	0.0
5	1.25	5	0.0	5	5	0.0
6	1.35	6	0.0	6	6	0.0
7	1.45	7	0.0	7	7	0.0
8	1.55	8	0.0	8	8	0.0
9	1.65	9	0.0	9	9	0.0
10	1.75	10	0.0	10	10	0.0

Assumption effects were calculated to be negligible.

DETERMINATION OF PARAMETERS

The atomic parameters listed by Broge for the compound cell were converted by graphical means to the coordinates in the primitive unit as follows:

	x	y	z
C ₁	-0.139	+0.044	-0.057
C ₂	-0.198	-0.024	-0.259
C ₃	-0.224	-0.266	-0.204
C ₄	-0.133	-0.170	0.000
F ₁	+0.220	-0.229	0.000
F ₂	-0.116	+0.115	-0.454
F ₃	-0.487	+0.030	-0.364
F ₄	-0.083	-0.415	-0.354
F ₅	-0.374	-0.479	-0.268
F ₆	-0.244	-0.354	+0.180

Figures 13 and 14 show projections on (010) and (100) of the reduced cell that would be obtained using the above. The centrosymmetric model is clearly outlined.

Amplitudes calculated from these positions however failed to agree with observed values. This indicated that the proposed structure was not close to the true one and that the experimental data should be used systematically in a search for the correct structure.

The atomic parameters listed by Rogers for the same
 point were converted by graphical means to the
 coordinates in the primitive cell as follows:

x	y	z	
-0.007	+0.004	-0.100	C1
-0.008	-0.004	-0.100	C2
-0.004	-0.004	-0.024	C3
0.000	-0.007	-0.100	C4
0.000	-0.008	+0.020	V1
-0.004	+0.008	-0.100	V2
-0.004	+0.000	-0.007	V3
-0.004	-0.008	-0.008	V4
-0.008	-0.007	-0.024	V5
-0.100	-0.004	-0.004	V6

Figures 13 and 14 show projections on (010) and (100)
 of the structure that would be obtained using the above.
 The centrosymmetric model is clearly outlined.
 Significant evidence from these positions however
 failed to agree with observed values. This indicated
 that the proposed structure was not close to the true
 one and that the experimental data should be used system-
 atically in a search for the correct structure.

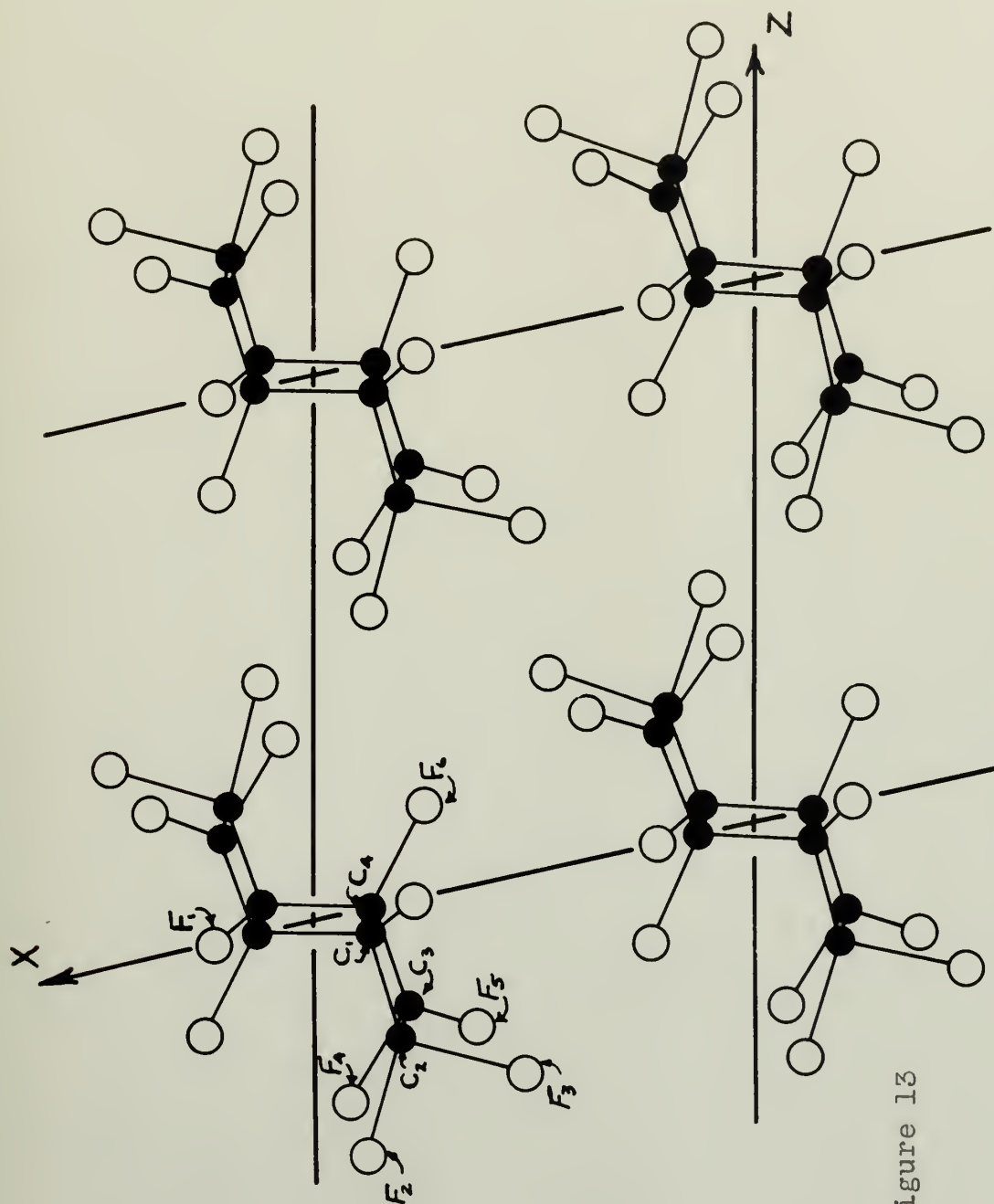
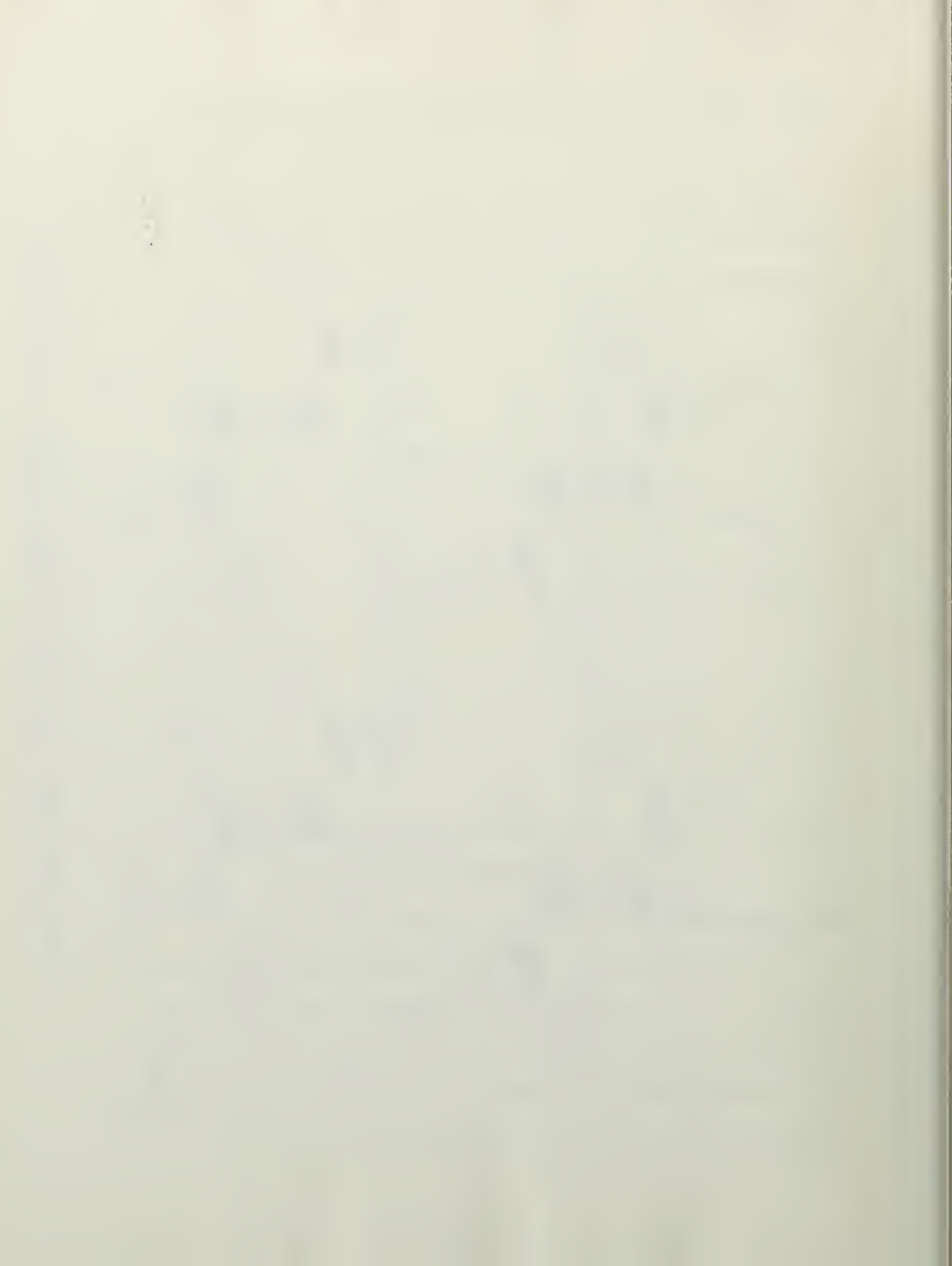


Figure 13

PROJECTION ON (010) FROM DATA OF BROGE



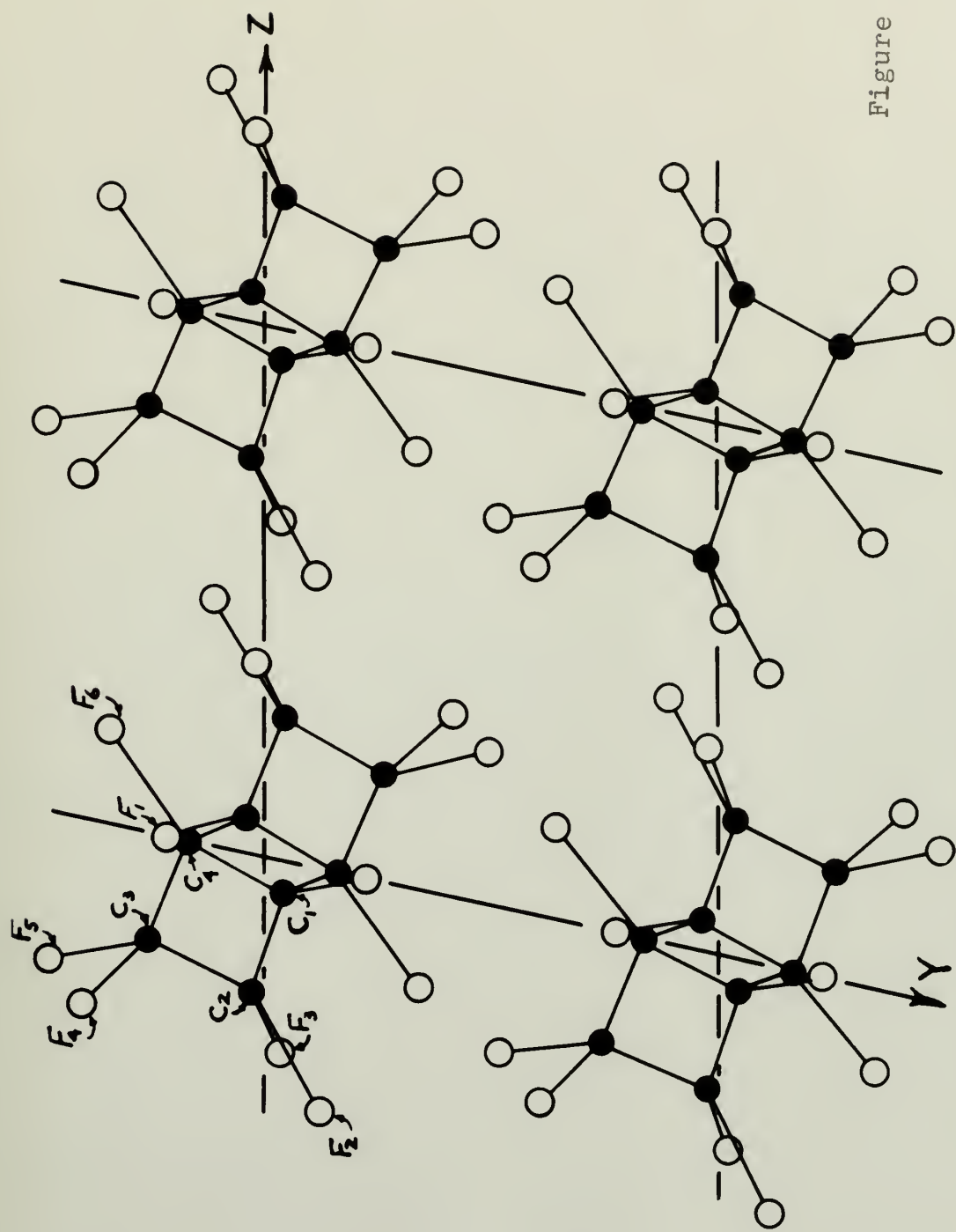


Figure 14

PROJECTION ON (100) FROM DATA OF BROGE

Patterson Projection, $P(Y,Z)$.

Since the first data were observed for rotation about a_1 the Patterson projection on (100) was computed. It can be shown that

$$\begin{aligned}
 KP(Y,Z) = & \sum_{k=0}^{\infty} \sum_{\ell=0}^{\infty} \left[|F_{0k\ell}|^2 + |F_{0\bar{k}\ell}|^2 \right] \cos 2 \pi k Y \cos 2 \pi \ell Z \\
 & - \sum_{k=1}^{\infty} \sum_{\ell=1}^{\infty} \left[|F_{0k\ell}|^2 - |F_{0\bar{k}\ell}|^2 \right] \sin 2 \pi k Y \sin 2 \pi \ell Z
 \end{aligned}$$

(neglecting constant additive terms).

The projection is shown in Figure 15. Contours start at 0 and are drawn at intervals of 50 in relative Patterson density. Aside from the identity peak at the origin, a single solid ridge is seen extending from $Y=0, Z=0$ to $Y=1, Z=-1/2$ with peaks at intervals along the entire length. This would lead one to believe that the long axis of the molecule lay parallel to the ridge. Further evidence lies in the fact that the (012) reflection is indicative of strong temperature diffuse scattering. The significance of such reflections is discussed by Lonsdale.⁽²²⁾ Trial parameters assigned to the atoms on the basis of such an orientation failed to give a satisfactory comparison of calculated and observed amplitudes for $F(00\ell)$ and $F(0k0)$.

pattern projection $P(Y, Z)$.

Since the first data were observed for rotation about z , the pattern projection on (100) was computed. It can be shown that

$$P(Y, Z) = \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \left[\frac{1}{2} (|x_{0k}|^2 + |x_{0l}|^2) \cos 2\pi k Y \cos 2\pi l Z \right]$$

$$- \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \left[\frac{1}{2} (|x_{0k}|^2 - |x_{0l}|^2) \sin 2\pi k Y \sin 2\pi l Z \right]$$

(neglecting constant additive terms).

The projection is shown in Figure 10. Contours start at 0 and are drawn at intervals of 50 in relative Patterson density. Aside from the identity peak at the origin, a single ridge is seen extending from $Y=0, Z=0$ to $Y=1, Z=1/2$ with peaks at intervals along the entire length. This would lead one to believe that the long axis of the molecule lay parallel to the ridge. Further evidence lies in the fact that the (011) reflection is indicative of strong temperature diffuse scattering. The slight-ness of such reflections is discussed by Lonsdale.⁽²²⁾ Total parameters assigned to the atoms on the basis of such an orientation failed to give a satisfactory comparison of calculated and observed amplitudes for $P(001)$ and $P(010)$.

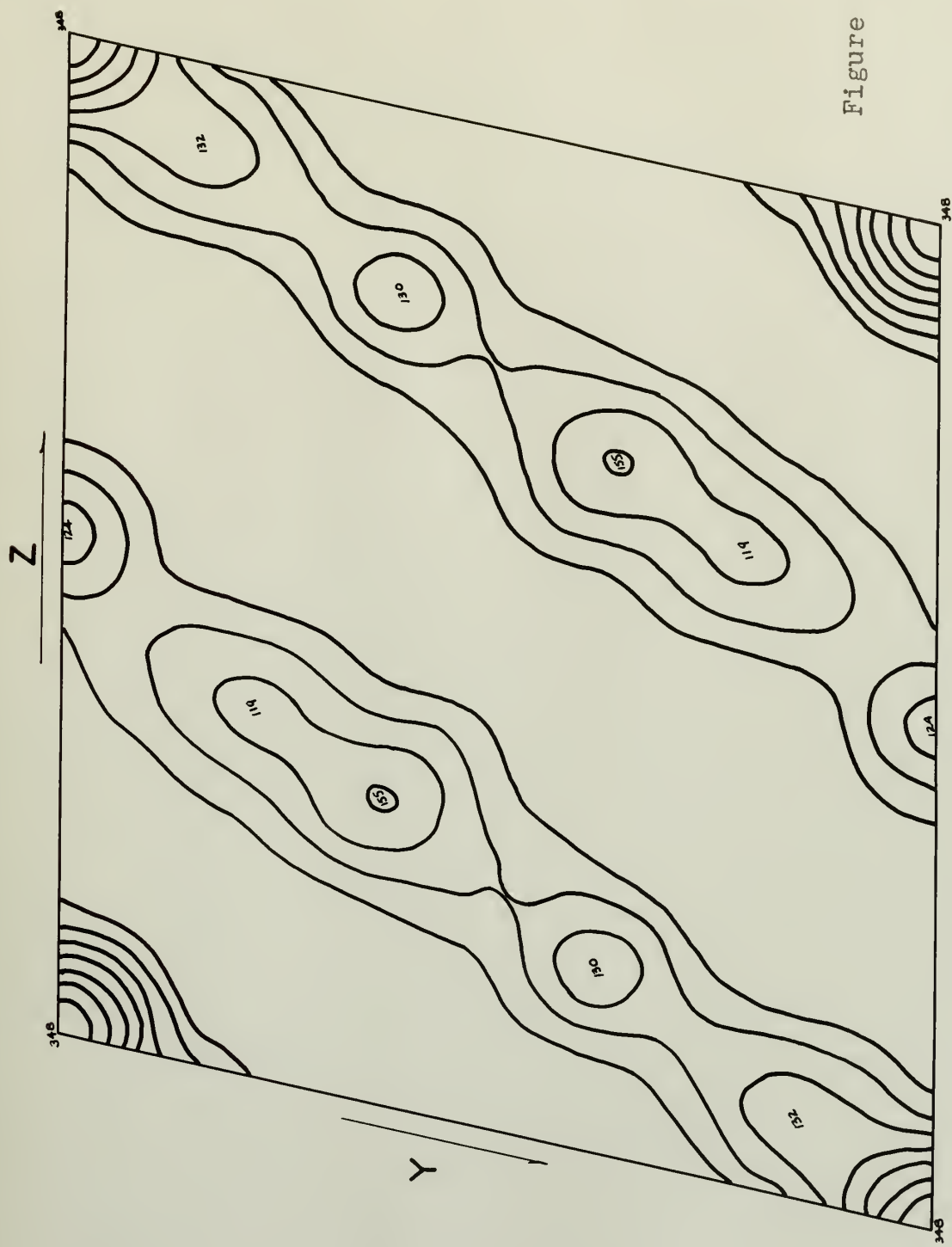


Figure 15

PATTERSON PROJECTION $P(Y,Z)$

Patterson Projection, $P(X,Z)$.

The function, apart from constant additive terms, may be expressed as:

$$\begin{aligned}
 KP(X,Z) = & \sum_{h=0}^{\infty} \sum_{\ell=0}^{\infty} \left[|F_{h0\ell}|^2 + |F_{\bar{h}0\ell}|^2 \right] \cos 2 \pi hX \cos 2 \pi \ell Z \\
 & - \sum_{h=1}^{\infty} \sum_{\ell=1}^{\infty} \left[|F_{h0\ell}|^2 - |F_{\bar{h}0\ell}|^2 \right] \sin 2 \pi hX \sin 2 \pi \ell Z.
 \end{aligned}$$

The projection on (010) of the primitive reduced cell is shown in Figure 16. Contours are drawn as before. Several isolated peaks appear and may be grouped along straight lines with striking regularity. Several orientations based on features of this projection were tried but failed to give satisfactory agreement of observed and calculated amplitudes.

Peaks arising from vectors between equivalent atoms will appear on $P(X,Z)$ at $X=2x, Z=2z$. A scaled model of the unit cell was made so that trial structures could be set up with cork balls to represent appropriate atoms. Even with the model it was not possible to determine which of the peaks appeared because of equivalent atoms. The parameters obtained from Broge's analysis were used to plot peaks at $2x, 2z$ on an overlay of the Patterson projection. The coordinates were adjusted to agree with the peaks on the projection and structure amplitudes

projection, $V(x, z)$.

The function, apart from constant additive terms,

may be expressed as:

$$V(x, z) = \sum_{n=0}^{\infty} \sum_{l=0}^{\infty} \frac{1}{n! l!} \left[\frac{\partial^2}{\partial x^2 \partial z^2} \right]^n \left[\frac{\partial^2}{\partial x^2 \partial z^2} \right]^l V(x, z)$$

$$= \sum_{n=0}^{\infty} \sum_{l=0}^{\infty} \frac{1}{n! l!} \left[\frac{\partial^2}{\partial x^2 \partial z^2} \right]^n \left[\frac{\partial^2}{\partial x^2 \partial z^2} \right]^l V(x, z)$$

The projection on (010) of the primitive reduced cell is shown in figure 1. Contours are drawn as before. Several isolated peaks appear and may be grouped along straight lines with striking regularity. Several extensions based on features of this projection were tried but failed to give satisfactory agreement of observed and calculated amplitudes.

Peaks arising from vectors between equivalent atoms will appear on $V(x, z)$ at $x=0, z=0$. A scaled model of the unit cell was made so that trial structures could be set up with cork balls to represent appropriate atoms. Even with the model it was not possible to determine which of the peaks appeared because of equivalent atoms. The parameters obtained from Broge's analysis were used to plot peaks at $2\pi, 2\pi$ on an overlay of the projection projection. The coordinates were adjusted to agree with the peaks on the projection and structure amplitudes

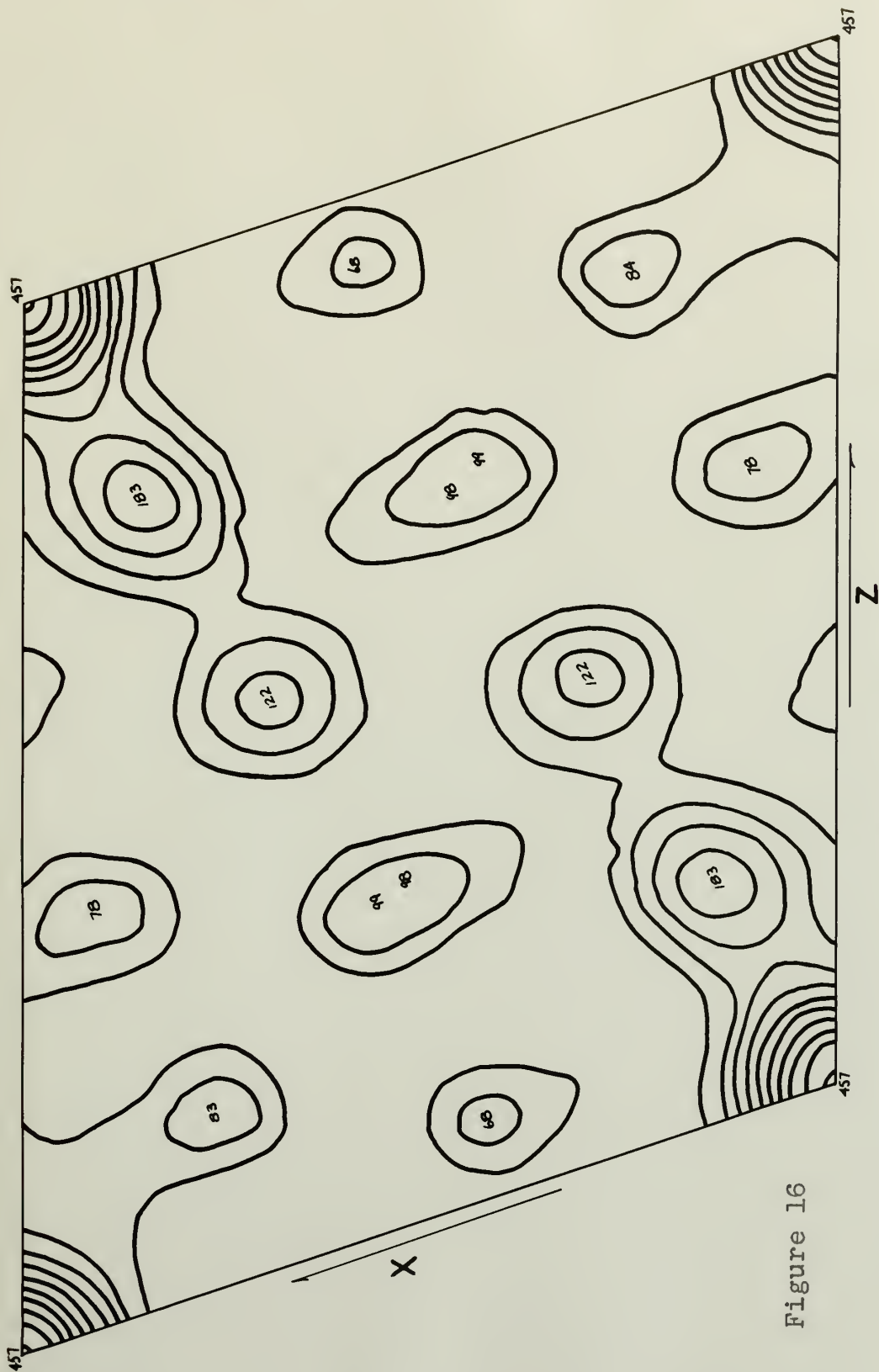


Figure 16

PATTERSON PROJECTION $P(XZ)$

computed. Again there was no agreement.

Since the ($\bar{2}21$) reflection was so very strong it was suspected that a large amount of scattering material was located in the corresponding plane. The Patterson density from $P(X,Z)$ was plotted on a properly drawn grid of the ($\bar{2}21$) plane. Any vectors between atoms lying in this plane would appear in their true length in the preceding plot. The scaled molecular model was placed in several orientations such that many of the fluorines lay in the plane. No vectors could be recognized however.

Patterson Projection, $P(X',Z')$.

The projection on the $a_1'' a_3''$ face of the unit cell of crystal #4 was calculated. This corresponds to $(01\bar{1})$ of the reduced unit. It is shown in Figure 17. Contours start at 0 and are drawn at intervals of 20 in arbitrary relative Patterson density. Here again there is a long ridge extending from $X'=0, Z'=0$ to $X'=1/2, Z'=1$ with poorly defined peaks all along the ridge. The plane of projection was properly fitted into the primitive reduced cell to see if three coordinates could be assigned to any one vector peak. This procedure failed to clarify the situation however.

computed. Again there was no agreement.

Since the (111) reflection was so very strong it was suspected that a large amount of scattering material was located in the corresponding plane. The Patterson density from $P(x, y)$ was plotted as a properly drawn grid of the (111) plane. Any vectors between atoms lying in this plane would appear in their true length in the projecting plot. The scaled molecular model was placed in several orientations such that many of the fluorine lay in the plane. No vectors could be recognized however.

Patterson projection, $P(x, y)$.

The projection on the xy face of the unit cell of crystal was calculated. This corresponds to (011) of the reduced unit. It is shown in Figure 17. Contours start at 0 and are drawn at intervals of 20 in arbitrary relative Patterson density. There again there is a long ridge extending from $x=0, y=0$ to $x=1/2, y=1/2$ with peaks lying along the ridge. The plane of projection was properly tilted into the perspective reduced cell so as to have coordinates could be assigned to any one vector peak. This procedure failed to clarify the situation however.

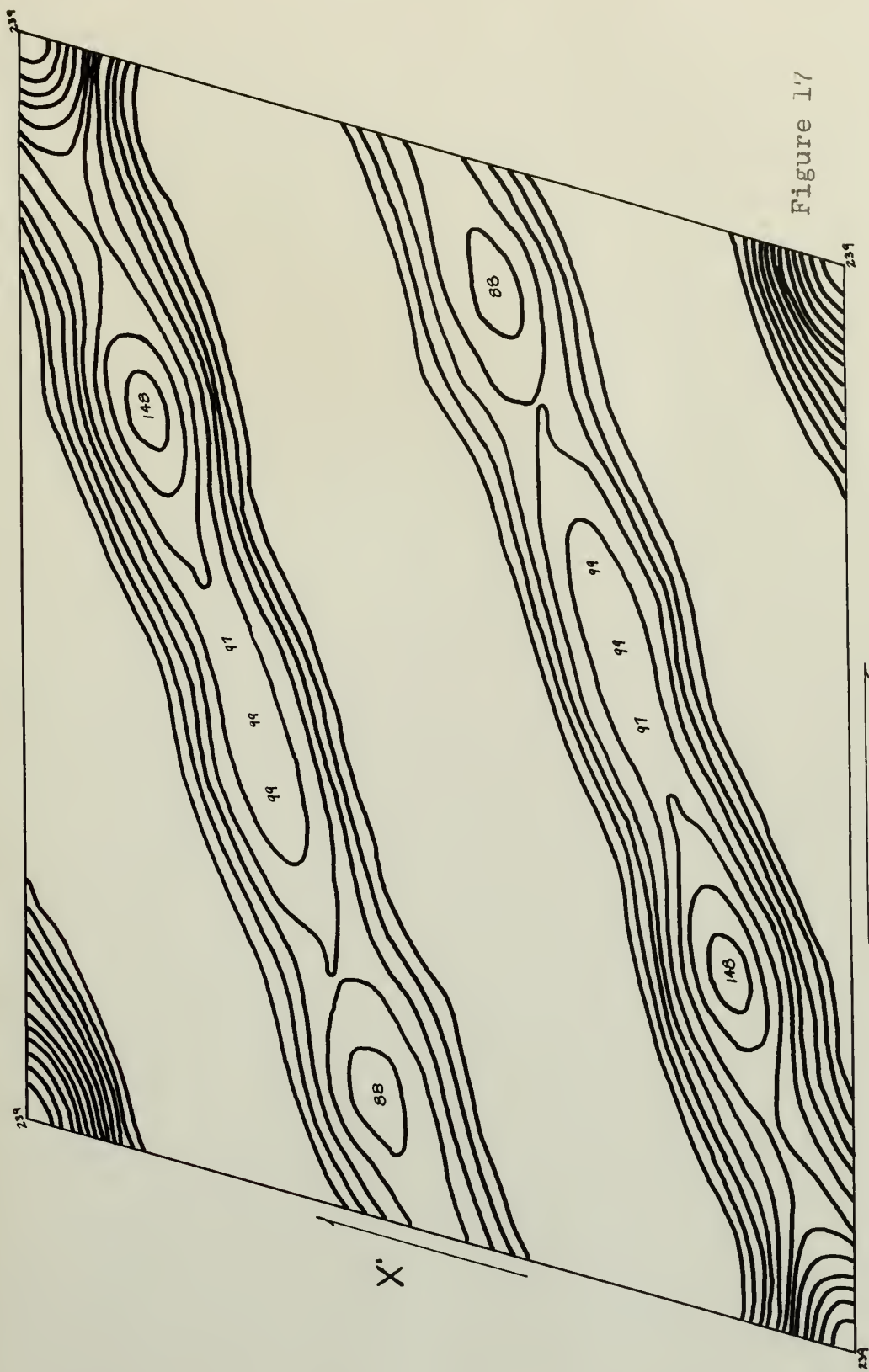


Figure 17

PATTERSON PROJECTION $P(X', Z')$

Phase Inequalities and Unitary Structure Amplitudes.

Since none of the projections were successfully interpreted, the possibility of phase determination by the recently proposed inequality procedure was explored. Unitary amplitudes are required in the inequality method and were, therefore, calculated for $(0k\ell)$ and $(h0\ell)$ data.

It was soon clear that only a few F's were greater than 0.5 and that there were certainly not enough of sufficiently high magnitude to determine more than a few phases. If the assumed model were correct, the method might be further exploited. However, if the center of symmetry is lost, the procedure no longer is applicable.

Temporary Conclusion of the Work

Thus far, all attempts at parameter determination had failed. It was at this point that C_4Cl_8 became available for study. It was decided that more would be accomplished in the long run if the C_8F_{12} problem were dropped at this time in order to determine the structure of the octachlorocyclobutane. Any knowledge gained concerning the configuration of the carbon ring in the latter compound might then lead to reconsideration of the proper model to use in work on the former.

Recently Professor Miller made available for study the compound $C_8Cl_4F_8$ analagous to C_8F_{12} wherein the

board inequalities and binary structure inequalities. Since some of the projections were successfully interpreted, the possibility of phase determination by the recently proposed inequality procedure was explored. Binary inequalities are reported in the inequality method and were, therefore, calculated for (001) and (100) data. It was also clear that only a few F^2 's were greater

than 0.2 and that there were certainly not enough of sufficiently high magnitude to determine more than a few phases. If the assumed model were correct, the method might be further exploited. However, if the center of symmetry is lost, the procedure no longer is applicable.

Temporary Conclusion of the Work

Thus far, all attempts at parameter determination had failed. It was at this point that C_{4v} became available for study. It was decided that more would be accomplished in the long run if the C_{4v} problem were dropped at this time in order to determine the structure of the octahedral complex. Any knowledge gained concerning the configuration of the cation ring in the latter compound might then lead to reconsideration of the proper model to use in work on the former.

Recently Professor Miller made available for study

the compound C_{4v} analogous to C_{4v} wherein the

fluorines attached to the central carbon ring have been replaced by chlorine atoms. It was at first believed that structure studies of this material might help in the solution of the hexafluorobutadiene dimer. Preliminary work has shown that crystals of the new compound have cubic symmetry and thus are not isomorphous with C_8F_{12} . There is, however, evidence of molecular rotation at room temperatures so further work at lower temperatures may give more information.

Fluorine attached to the central carbon they have been replaced by chlorine atoms. It was at first believed that structural studies of this material might help in the solution of the hexafluorobenzene puzzle. Further study has shown that crystals of the new compound have cubic symmetry and thus are not isomorphous with C₆F₆. There is, however, evidence of retained rotation at room temperature so further work at lower temperatures may give more information.

SUGGESTIONS FOR FURTHER STUDY

In view of the evidence of the non-planar carbon ring in C_4Cl_8 it may be possible that the rings in C_8F_{12} are puckered with a resulting loss of a center of symmetry for the molecule. If this be true, the structure problem will be extremely difficult but not impossible.

Nearly complete $(hk\ell)$ data have been obtained for the primitive reduced cell. It is thus possible to calculate a series of three-dimensional Patterson sections for small increments along a chosen axis, probably a_2 . From these sections enough vectors might be resolved to lead to a satisfactory structure determination.

resolved to lead to a satisfactory structure determination. From these sections enough vectors might be taken for small fragments along a chosen axis, perpendicular to a series of three-dimensional patterns and the relative reduced cells. It is thus possible to locate specific points (as data have been obtained for the structure).

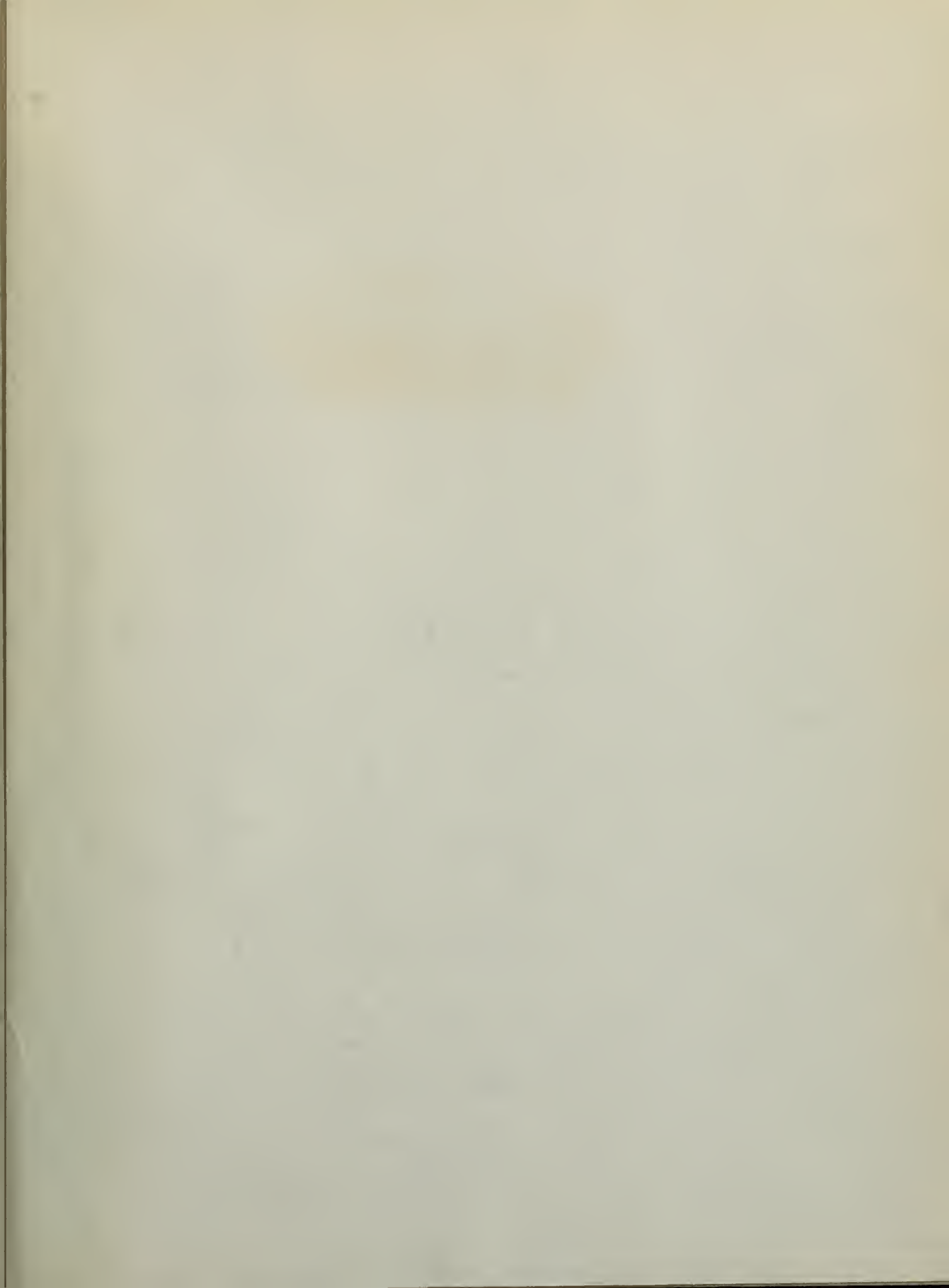
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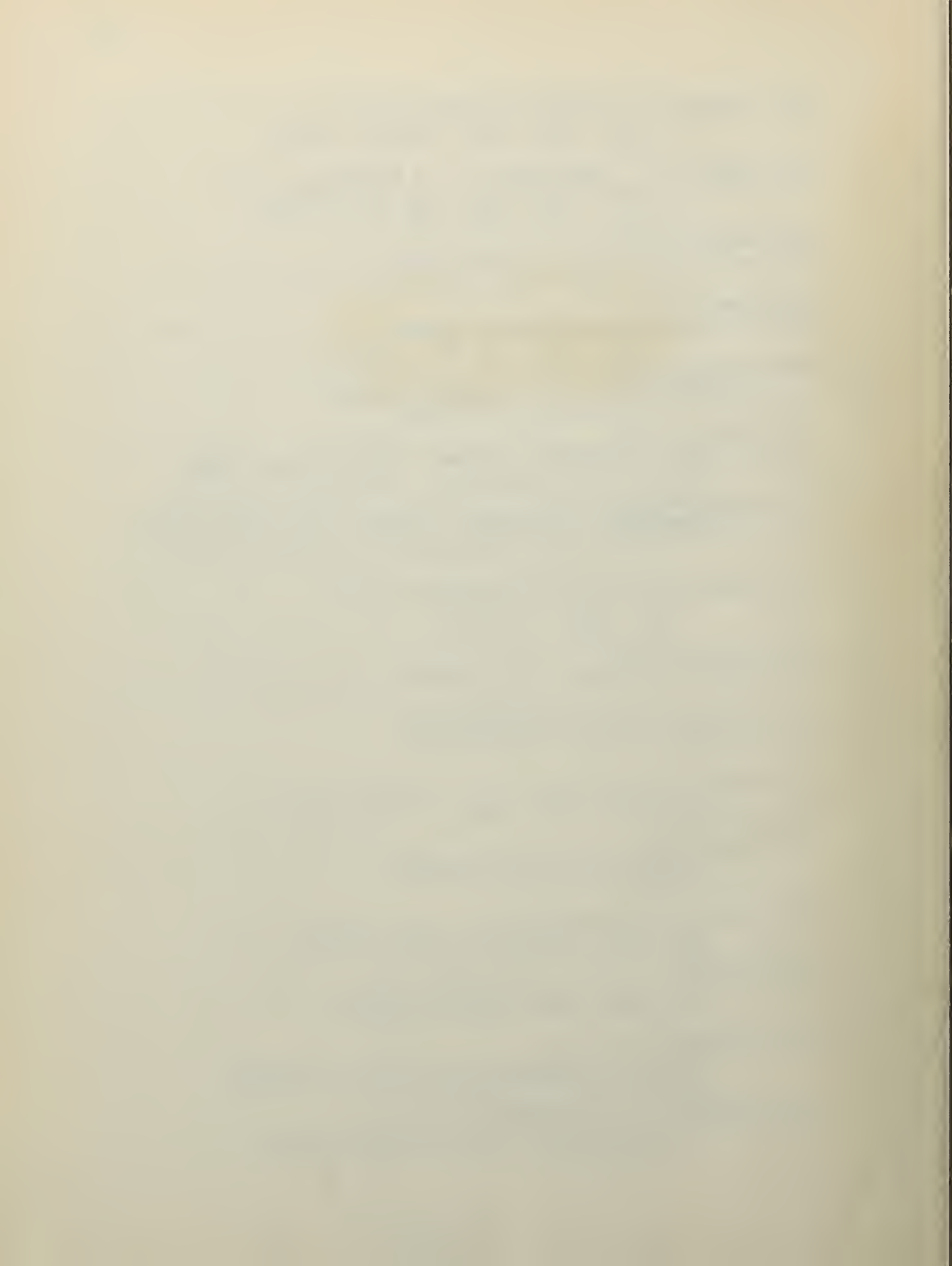
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I. The structure of
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of C₈F₁₂.

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